



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 146707

**TO:** Rei-Tsang Shiao  
**Location:** 5a10 / 5c18  
**Monday, March 14, 2005**  
**Art Unit:** 1626  
**Phone:** 571-272-0707  
**Serial Number:** 10 / 622130

**From:** Jan Delaval  
**Location:** Biotech-Chem Library  
**Remsen 1a51**  
**Phone:** 571-272-22504  
  
**[jan.delaval@uspto.gov](mailto:jan.delaval@uspto.gov)**

### Search Notes

*In behavioral  
for search*

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Bob) Shaw Examiner #: 79521 Date: 7/3/05  
 Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/622 130  
 Mail Box and Bldg/Room Location: 5A17c 18 Results Format Preferred (circle): PAPER  DISK  E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

*# any question please call me*

Title of invention: Heterodiamondoids at 2-0707

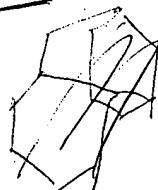
Inventors (please provide full names): Lia et al

Earliest Priority Filing Date:

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I Search a heterodiamondoid compound have  
 a diamondoid nucleus selected from trimantane  
 or tetramantane nucleus, and the nucleus  
 has a atom selected from N, S, O  
 (see Fig1, 5, 6, 7, 8)

II Search a compound (see Frs 2), of the ring structure  
 and one of carbon atoms is replaced by  
 N, O, S, Se, B, P, As



## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>John</u>	NA Sequence (#) <input checked="" type="checkbox"/>	STN <input checked="" type="checkbox"/>
Searcher Phone #: <u>23604</u>	AA Sequence (#) <input type="checkbox"/>	Dialog <input type="checkbox"/>
Searcher Location: <u>310 (05</u>	Structure (#) <input checked="" type="checkbox"/>	Questel/Orbit <input type="checkbox"/>
Date Searcher Picked Up: <u>3104/05</u>	Bibliographic <input type="checkbox"/>	Dr. Link <input type="checkbox"/>
Date Compiled: <u>3104/05</u>	Litigation <input type="checkbox"/>	Lexis/Nexis <input type="checkbox"/>
Searcher Prep: Review Time <u>3:13</u>	Fulltext <input type="checkbox"/>	Sequence Systems <input type="checkbox"/>
Clerical Prep: time: <u>+ 90</u>	Patent Family <input type="checkbox"/>	WWW/Internet <input type="checkbox"/>
Online Time	Other <input type="checkbox"/>	Other (specify) _____

=> d his

(FILE 'HOME' ENTERED AT 09:27:34 ON 10 MAR 2005)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:27:42 ON 10 MAR 2005  
L1 1 S US20040059145/PN OR (US2003-622130# OR WO2003-US22483 OR US20  
E HETERODIAMON  
L2 23 S E4-E7  
E CHEVRON/PA,CS  
L3 5478 S CHEVRON?/PA,CS  
E CHEVRO/PA,CS  
E LIU S/AU  
L4 528 S E3,E12  
E LIU SHENG/AU  
L5 148 S E3,E16  
E LIU SHENGGAO/AU  
L6 22 S E3  
E CARLSON R/AU  
L7 88 S E3,E17,E18  
E CARLSON ROB/AU  
L8 163 S E4,E21-E25  
E DAHL J/AU  
L9 24 S E3,E7,E8  
E DAHL JEREMY/AU  
L10 32 S E3-E7  
L11 77 S ?TETRAMANTAN? OR ?TRIAMANTAN?  
L12 263 S ?DIAMONDOID?  
L13 3 S L1,L3-L10 AND L2  
L14 21 S L1,L3-L10 AND L11,L12  
L15 21 S L13,L14  
L16 5 S L15 AND ?ADAMANTAN?  
L17 13 S L15 AND ?AMANTAN?  
L18 13 S L16,L17  
L19 8 S L15 NOT L18  
L20 41 S L15-L19,L2  
L21 37 S L12 AND L11  
L22 98 S L12 AND ?AMANTAN?  
L23 98 S L21,L22

FILE 'REGISTRY' ENTERED AT 09:35:31 ON 10 MAR 2005

FILE 'HCAPLUS' ENTERED AT 09:35:31 ON 10 MAR 2005

SET SMARTSELECT ON

L24 SEL L23 1- RN : 796 TERMS  
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 09:35:34 ON 10 MAR 2005

L25 796 S L24  
L26 401 S L25 AND NR>=5  
L27 359 S L26 NOT HYDROCARBON  
L28 80 S L27 AND ?AMANTAN?/CNS  
L29 59 S L28 NOT C6-C6-C6/ES  
L30 38 S L29 AND (SE OR AS OR B OR AL OR SI OR N OR P OR O OR S)/ELS  
L31 16 S L30 AND (C15H20O2 OR C16H20O4 OR C14H200 OR C18H220 OR C18H26  
L32 22 S L30 NOT L31  
L33 42 S L28 NOT L30  
L34 279 S L27 NOT L28-L33  
L35 0 S L34 AND ?MANTAN?/CNS  
L36 24 S L34 AND (C18H24GE2 OR C21H27P OR C22H27NO OR C21H27N OR C20H2  
L37 29 S L34 AND (C21H26S3 OR C23H30O2 OR C20H24SI2 OR C13H19B OR C18H  
L38 40 S L36,L37  
L39 5 S L38 AND (CARBOXYLIC OR C21H26O)

SEL RN 4 5  
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L41 3 S L39 NOT L40  
L42 37 S L38 NOT L41  
L43 42 S L26 NOT L27  
L44 59 S L32,L42  
SAV L44 SHIAO622/A  
L45 STR  
L46 21 S L45  
L47 STR L45  
L48 0 S L47  
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L50 0 S L49  
L51 STR L49  
L52 SCR 1843  
L53 0 S (L47 OR L49 OR L51) AND L52 SAM  
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BATCH L57 SHIAO622A/B SSS FULL

FILE 'HCAOLD' ENTERED AT 10:22:33 ON 10 MAR 2005  
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FILE 'HCAPLUS' ENTERED AT 10:22:37 ON 10 MAR 2005  
L62 4 S L44  
L63 3 S L62 AND L1-L23  
L64 4 S L62,L63

FILE 'USPATFULL' ENTERED AT 10:23:27 ON 10 MAR 2005  
L65 1 S L44

=> fil uspatful  
FILE 'USPATFULL' ENTERED AT 10:23:48 ON 10 MAR 2005  
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 8 Mar 2005 (20050308/PD)  
FILE LAST UPDATED: 8 Mar 2005 (20050308/ED)  
HIGHEST GRANTED PATENT NUMBER: US6865747  
HIGHEST APPLICATION PUBLICATION NUMBER: US2005050605  
CA INDEXING IS CURRENT THROUGH 8 Mar 2005 (20050308/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 8 Mar 2005 (20050308/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
>>> original, i.e., the earliest published granted patents or <<<  
>>> applications. USPAT2 contains full text of the latest US <<<  
>>> publications, starting in 2001, for the inventions covered in <<<  
>>> USPATFULL. A USPATFULL record contains not only the original <<<  
>>> published document but also a list of any subsequent <<<  
>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
>>> records and may be searched in standard search fields, e.g., /PN, <<<  
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<  
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<

>>> enter this cluster.  
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 >>> Use USPATALL when searching terms such as patent assignees,  
 >>> classifications, or claims, that may potentially change from  
 >>> the earliest to the latest publication.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 165 bib abs hitstr

L65 ANSWER 1 OF 1 USPATFULL on STN  
 AN 2004:77366 USPATFULL  
 TI Heterodiamondoids  
 IN Liu, Shenggao, Hercules, CA, UNITED STATES  
     Carlson, Robert M., Petaluma, CA, UNITED STATES  
     Dahl, Jeremy E., Palo Alto, CA, UNITED STATES  
 PA CHEVRON USA INC. (U.S. corporation)  
 PI US 2004059145 A1 20040325  
 AI US 2003-622130 A1 20030716 (10)  
 PRAI US 2002-397367P 20020718 (60)  
 DT Utility  
 FS APPLICATION  
 LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404,  
     Alexandria, VA, 22313-1404  
 CLMN Number of Claims: 37  
 ECL Exemplary Claim: 1  
 DRWN 51 Drawing Page(s)  
 LN.CNT 2469

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention is related to heteroatom containing diamondoids (i.e., "heterodiamondoids") which are compounds having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compounds carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices can serve as optically active materials.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

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     [121212121] Thiadecamantane 652998-92-0, [121212121]  
     Selenadecamantane 652998-93-1, [121212121] Boradecamantane  
     652998-94-2, [121212121] Azadecamantane 652998-95-3,  
     [121212121] Phosphadecamantane 652998-96-4, [121212121]  
     Arsa decamantane 652998-98-6, [1212121212] Oxaundecamantane  
     652998-99-7, [1212121212] Thiaundecamantane 652999-00-3  
     , [1212121212] Selenaundecamantane 652999-01-4, [1212121212]  
     Boraundecamantane 652999-02-5, [1212121212] Azaundecamantane  
     652999-03-6, [1212121212] Phosphaundecamantane  
     652999-04-7, [1212121212] Arsaundecamantane 652999-05-8  
     652999-06-9 652999-08-1 652999-09-2  
     652999-11-6 652999-12-7 652999-35-4  
     652999-36-5 652999-38-7 652999-39-8  
     652999-40-1, [121212121] Boradecamantane 652999-41-2,  
     [121212121] Azadecamantane 652999-42-3, [121212121]  
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     652999-44-5, [1212121212] Boraundecamantane 652999-45-6

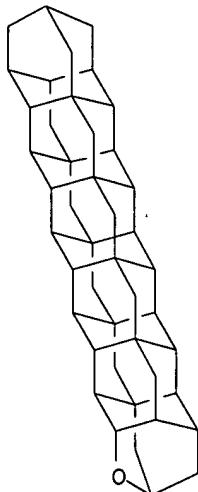
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Arsaundecamantane

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

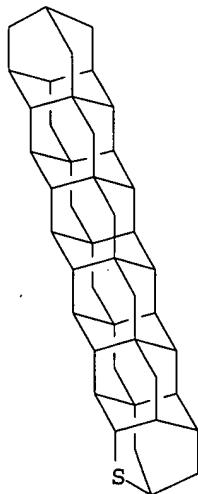
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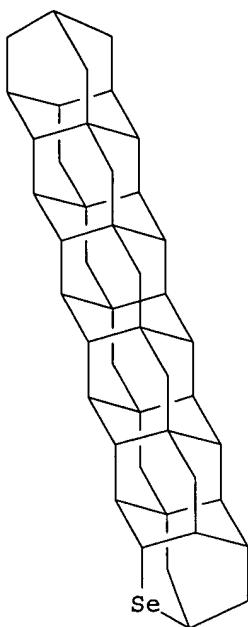
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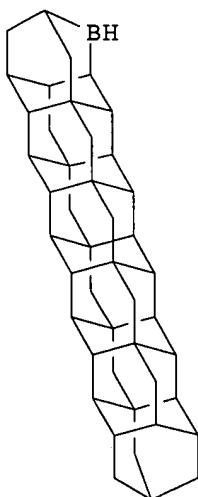


RN 652998-92-0 USPATFULL

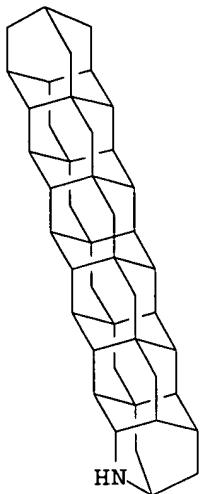
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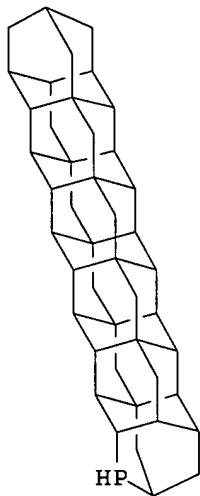
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CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



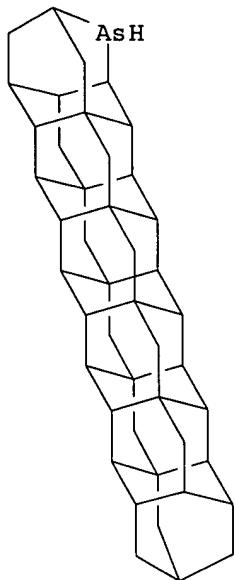
RN 652998-94-2 USPATFULL  
CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



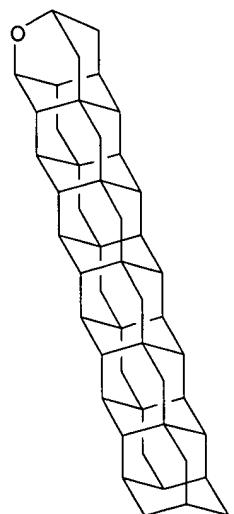
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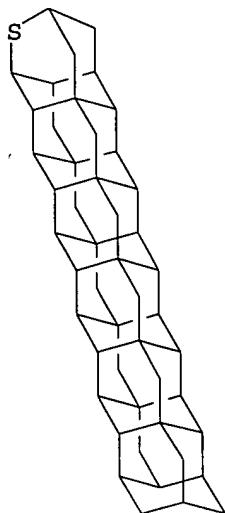
RN 652998-96-4 USPATFULL  
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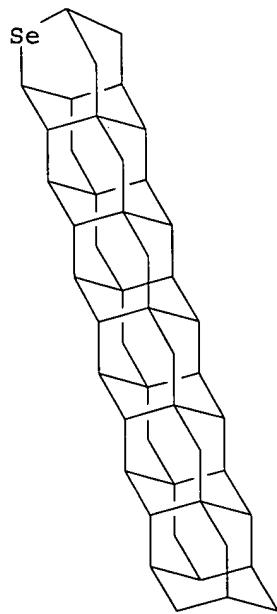
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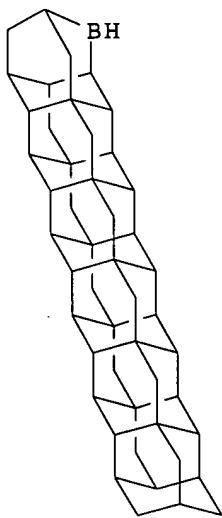
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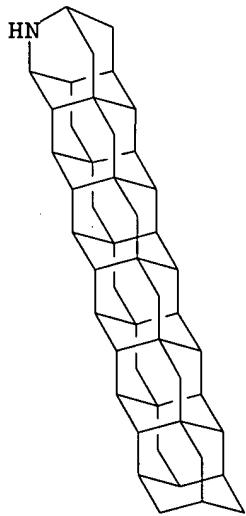
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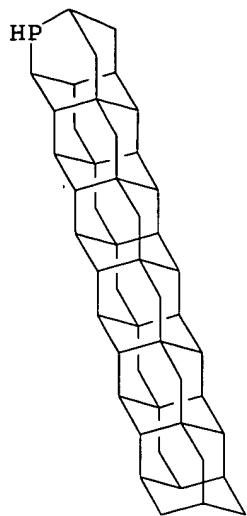
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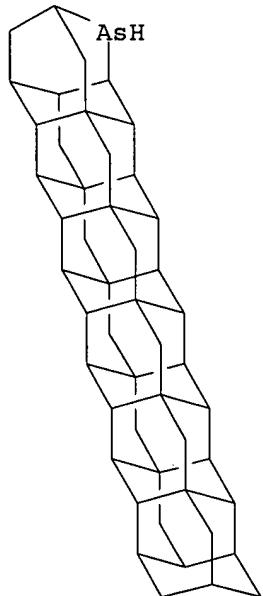
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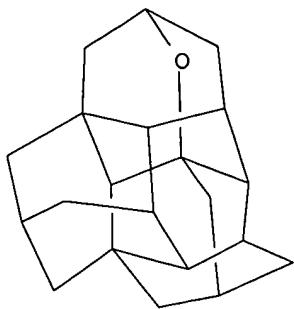
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RN 652999-04-7 USPATFULL  
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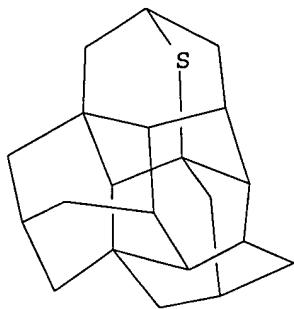


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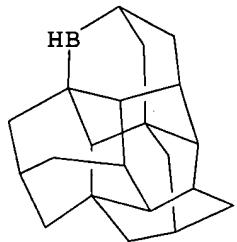
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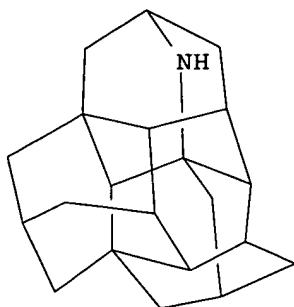
RN 652999-08-1 USPATFULL

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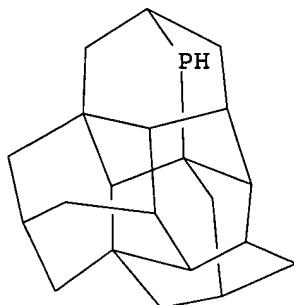
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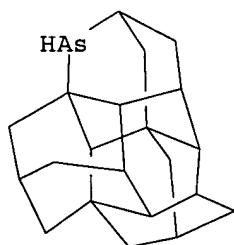
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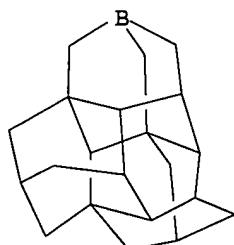
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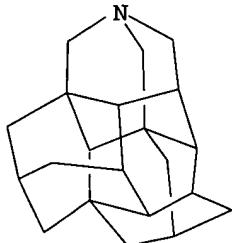
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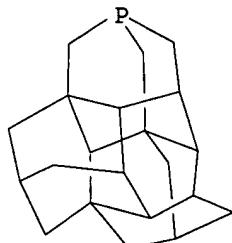
RN 652999-36-5 USPATFULL

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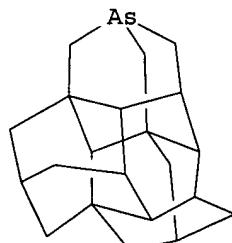
RN 652999-38-7 USPATFULL

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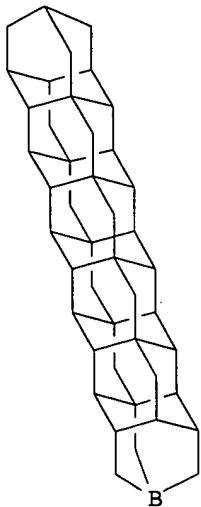
RN 652999-39-8 USPATFULL

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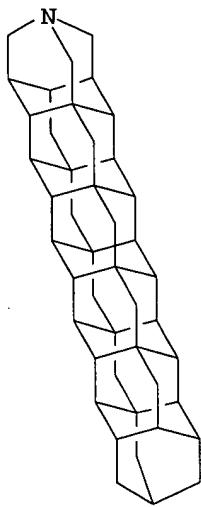


RN 652999-40-1 USPATFULL

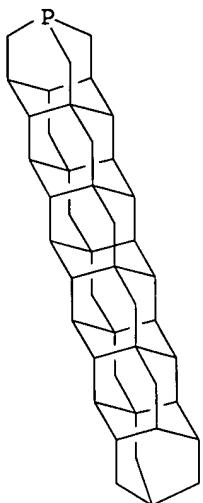
CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



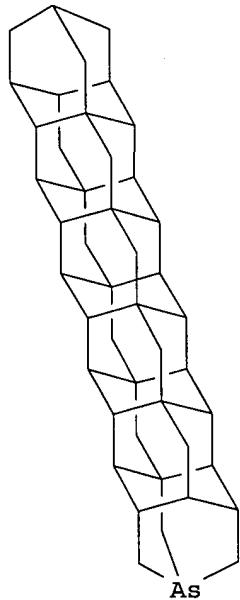
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CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



RN 652999-42-3 USPATFULL  
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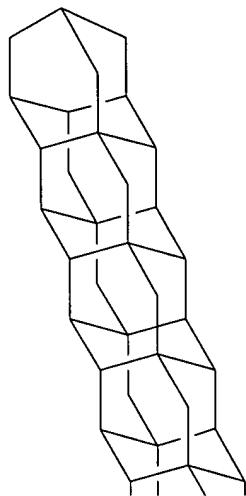


RN 652999-43-4 USPATFULL  
CN [121212121] Arsadecamantane (9CI) (CA INDEX NAME)

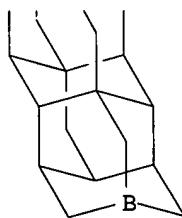


RN 652999-44-5 USPATFULL  
CN [1212121212] Boraundecamantane (9CI) (CA INDEX NAME)

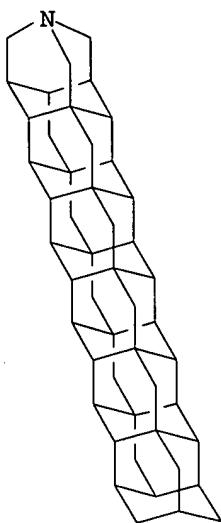
PAGE 1-A



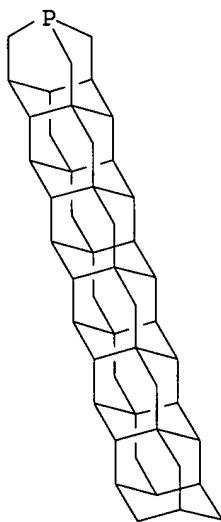
PAGE 2-A



RN 652999-45-6 USPATFULL  
CN [1212121212] Azaundecamantane (9CI) (CA INDEX NAME)

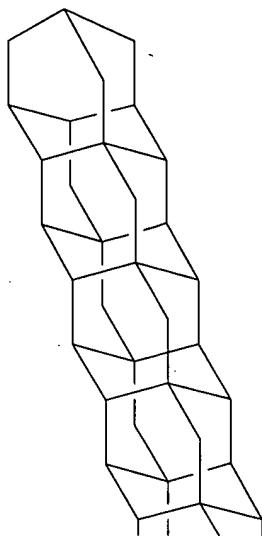


RN 652999-46-7 USPATFULL  
CN [1212121212] Phosphaundecamantane (9CI) (CA INDEX NAME)

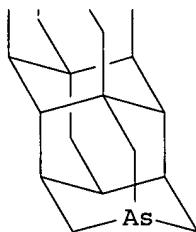


RN 652999-47-8 USPATFULL  
CN [1212121212] Arsaundecamantane (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

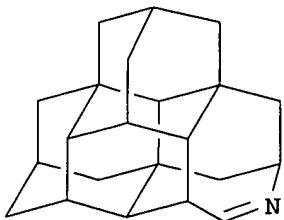


IT 652999-16-1P 652999-17-2P 652999-18-3P  
652999-19-4P 652999-20-7P 652999-23-0P  
652999-24-1P 652999-25-2P

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane  
from fused adamantanes such as tetramantanes)

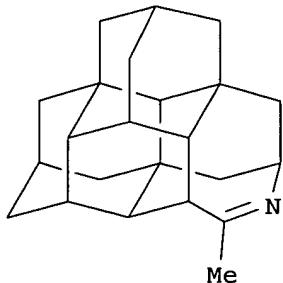
RN 652999-16-1 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA  
INDEX NAME)



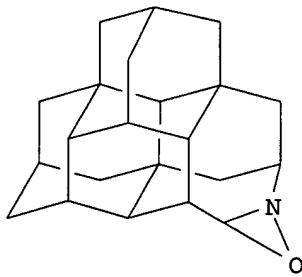
RN 652999-17-2 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro-1-methyl-(9CI) (CA INDEX NAME)



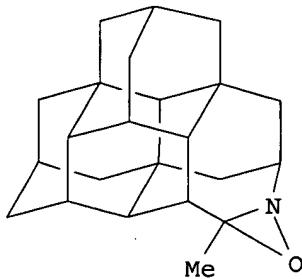
RN 652999-18-3 USPATFULL

CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro- (9CI) (CA INDEX NAME)



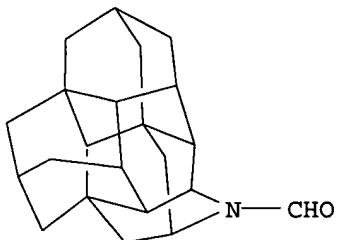
RN 652999-19-4 USPATFULL

CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro-12c-methyl- (9CI) (CA INDEX NAME)



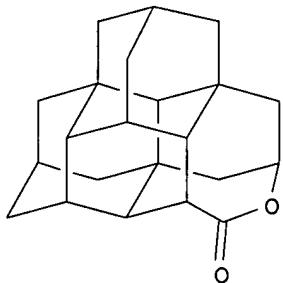
RN 652999-20-7 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline-1-carboxaldehyde, dodecahydro- (9CI) (CA INDEX NAME)



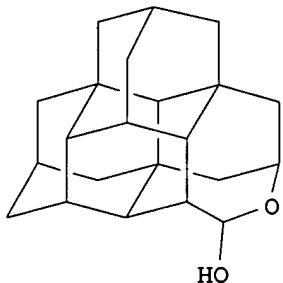
RN 652999-23-0 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-one, dodecahydro- (9CI) (CA INDEX NAME)



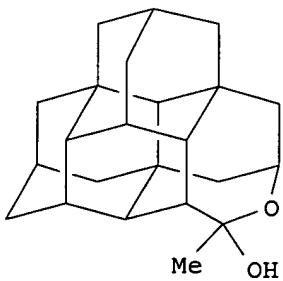
RN 652999-24-1 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-25-2 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)

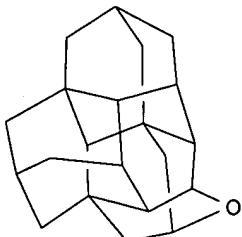


IT 652999-15-0P 652999-21-8P 652999-32-1P

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

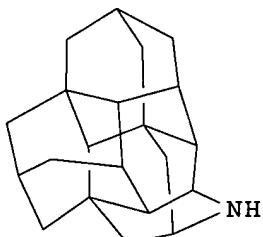
RN 652999-15-0 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran, dodecahydro- (9CI) (CA INDEX NAME)



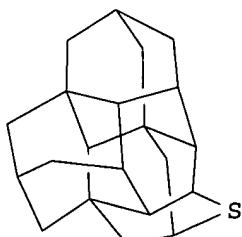
RN 652999-21-8 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-32-1 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



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FILE LAST UPDATED: 9 Mar 2005 (20050309/ED)

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L64 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:641668 HCAPLUS  
DN 141:320341  
ED Entered STN: 10 Aug 2004  
TI Diamond fragments as building blocks of functional nanostructures  
AU McIntosh, Gregory C.; Yoon, Mina; Berber, Savas; Tomanek, David  
CS Naval Base, Defence Technology Agency, Auckland, N. Z.  
SO Physical Review B: Condensed Matter and Materials Physics (2004), 70(4), 045401/1-045401/8  
CODEN: PRBMDO; ISSN: 0163-1829  
PB American Physical Society  
DT Journal  
LA English  
CC 65-3 (General Physical Chemistry)  
AB Using d. functional theory, we investigate the equilibrium structure, stability, and electronic properties of nanostructured, hydrogen-terminated diamond fragments. The equilibrium atomic arrangement and electronic structure of these nanostructures turn out to be very similar to bulk diamond. We find that such **diamondoids** may enter spontaneously into carbon nanotubes. Polymerization inside a nanotube is favored especially when boron and nitrogen are substituted for carbon atoms.  
ST **diamondoid** nanostructure electronic structure stability  
IT LUMO (molecular orbital)  
    (HOMO gap; diamond fragments as building blocks of functional nanostructures studied by DFT)  
IT HOMO (molecular orbital)  
    (LUMO gap; diamond fragments as building blocks of functional nanostructures studied by DFT)  
IT Bond length  
    (carbon-carbon; diamond fragments as building blocks of functional nanostructures studied by DFT)  
IT Nanotubes  
    (carbon; diamond fragments as building blocks of functional nanostructures studied by DFT)  
IT Band gap  
Band structure  
Binding energy  
Cluster model  
Conduction band  
Density of states  
Electron density  
HOMO (molecular orbital)  
LUMO (molecular orbital)  
Nanostructures  
Polymerization  
Valence band

(diamond fragments as building blocks of functional nanostructures studied by DFT)

IT Energy

(formation; diamond fragments as building blocks of functional nanostructures studied by DFT)

IT 281-23-2, Adamantane 2292-79-7, Diamantane

7782-40-3, Diamond, properties 27745-90-0, Tetramantane

112761-65-6, Decamantane 765943-15-5

765943-16-6

RL: PRP (Properties)

(diamond fragments as building blocks of functional nanostructures studied by DFT)

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 765943-15-5 765943-16-6

RL: PRP (Properties)

(diamond fragments as building blocks of functional nanostructures studied by DFT)

RN 765943-15-5 HCPLUS

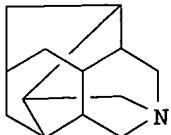
CN 1H-2,8,4,6-[1,2,3,4]Butanetetrayl-2-benzoborin, octahydro- (9CI) (CA INDEX NAME)



RN 765943-16-6 HCPLUS

CN 1H-2,8,4,6-[1,2,3,4]Butanetetraylisoquinoline, octahydro- (9CI) (CA INDEX)

NAME)



L64 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2004:365485 HCAPLUS  
 DN 141:318401  
 ED Entered STN: 05 May 2004  
 TI Theoretical analysis of diamond mechanosynthesis. Part II. C2 mediated growth of diamond C(110) surface via Si/Ge-triadamantane dimer placement tools  
 AU Mann, David J.; Peng, Jingping; Freitas, Robert A., Jr.; Merkle, Ralph C.  
 CS Zyvex Corp., Richardson, TX, 75081, USA  
 SO Journal of Computational and Theoretical Nanoscience (2004), 1(1), 71-80  
 CODEN: JCTNAB; ISSN: 1546-1955  
 PB American Scientific Publishers  
 DT Journal  
 LA English  
 CC 57-8 (Ceramics)  
 Section cross-reference(s): 66, 75  
 AB This paper presents a computational and theor. investigation of the vacuum mechanosynthesis of diamond on the clean C(110) surface from carbon dimer (C2) precursors positionally constrained throughout the reaction pathway by silicon- or germanium-doped triadamantane derivs. mounted on a scanning probe tip. Interactions between the dimer placement tools and the bare diamond C(110) surface are investigated using D. Functional Theory (DFT) with generalized gradient approximation (GGA) by constructing the reaction path potential energy profiles and analyzing ab initio mol. dynamics simulations. Similar methods are applied to study the energetics and kinetics of recharging the tool with acetylene. Mol. mechanics simulations on extended tool tips are carried out to elucidate the positional uncertainty of the carbon dimer due to thermal fluctuations, and the possibility of intermol. dimerization and dehydrogenation of the dimer placement tools is explored.  
 ST diamond growth dicarbon precursor  
 IT Simulation and Modeling, physicochemical  
     (mol. dynamics; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)  
 IT Reaction mechanism  
     (surface; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)  
 IT Mechanochemical reaction  
     Surface structure  
     (theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)  
 IT 7782-40-3, Diamond, processes  
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
     (theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)  
 IT 681029-68-5 681029-69-6  
     RL: PRP (Properties)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.  
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement  
tools)

IT 12070-15-4, Carbon dimer

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.  
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement  
tools)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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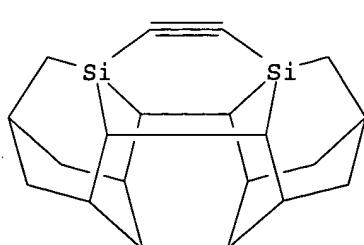
IT 681029-68-5 681029-69-6

RL: PRP (Properties)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.  
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement  
tools)

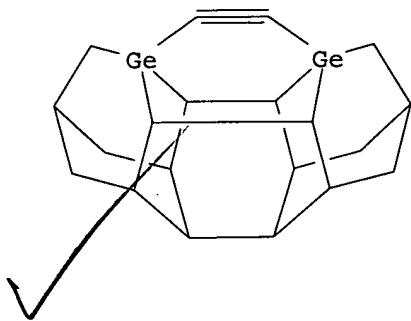
RN 681029-68-5 HCPLUS

CN Disila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



RN 681029-69-6 HCPLUS

CN Digerma[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



L64 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2004:80675 HCAPLUS  
 DN 140:146009  
 ED Entered STN: 01 Feb 2004  
 TI Preparation of heterodiamondoids from fused adamantanes  
 IN Liu, Shenggao; Carlson, Robert M.  
 PA Chevron U.S.A. Inc., USA; Dahl, Jeremy E.  
 SO PCT Int. Appl., 134 pp.  
 CODEN: PIXXD2

*SM*

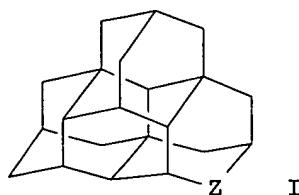
DT Patent  
 LA English  
 IC ICM C07D311-78  
 ICS C07D313-06; C07D335-04; C07D221-18  
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 76

FAN.CNT 1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004009577	A1	20040129	WO 2003-US22483	20030717 <--	
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004059145	A1	20040325	US 2003-622130	20030716 <--
PRAI US 2002-397367P	P	20020718			
US 2002-397368P	P	20020718			

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
	ICS	C07D313-06; C07D335-04; C07D221-18
US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C

OS MARPAT 140:146009  
 GI



- AB This invention is related to heteroatom containing **diamondoids** (i.e., 'heterodiamondoids'), e.g. **azatetramantane**, **oxatetramantane**, and **thiatetramantane** (I; X = NH, O, S), which are compds. having a **diamondoid** nucleus in which one or more of the **diamondoid** nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the **diamondoid**. In addition, the **heterodiamondoids** are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized **heterodiamondoids**. In a preferred aspect of this invention the **diamondoid** nuclei are **triemannane** and higher **diamondoid** nuclei. In another preferred aspect, the heteroatoms are selected to give rise to **diamondoid** materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).
- ST **heterodiamondoid prepn; azatetramantane**  
**oxatetramantane thiatetramantane prepn**
- IT Formation enthalpy  
(preparation of **heterodiamondoids** such as **aza-**, **oxa-**, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)
- IT Heterocyclic compounds  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of **heterodiamondoids** such as **aza-**, **oxa-**, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)
- IT 652998-89-5, [121212121] **Decamantane** 652998-90-8,  
[121212121] **Oxadecamantane** 652998-91-9, [121212121]  
**Thiadecamantane** 652998-92-0, [121212121]  
**Selenadecamantane** 652998-93-1, [121212121]  
**Boradecamantane** 652998-94-2, [121212121]  
**Azadecamantane** 652998-95-3, [121212121]  
**Phosphadecamantane** 652998-96-4, [121212121]  
**Arsadecamantane** 652998-97-5, [121212121] **Undecamantane**  
652998-98-6, [121212121] **Oxaundecamantane**  
652998-99-7, [121212121] **Thiaundecamantane**  
652999-00-3, [121212121] **Selenaundecamantane**  
652999-01-4, [121212121] **Boraundecamantane**  
652999-02-5, [121212121] **Azaundecamantane**  
652999-03-6, [121212121] **Phosphaundecamantane**  
652999-04-7, [121212121] **Arsaundecamantane**  
652999-05-8 652999-06-9 652999-07-0  
652999-08-1 652999-09-2 652999-11-6  
652999-12-7 652999-35-4 652999-36-5  
652999-38-7 652999-39-8 652999-40-1,  
[121212121] **Boradecamantane** 652999-41-2, [121212121]  
**Azadecamantane** 652999-42-3, [121212121]  
**Phosphadecamantane** 652999-43-4, [121212121]  
**Arsadecamantane** 652999-44-5, [121212121]  
**Boraundecamantane** 652999-45-6, [121212121]  
**Azaundecamantane** 652999-46-7, [121212121]

**phosphaundecamantane 652999-47-8, [1212121212]**

**Arsaundecamantane**

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 917-54-4, Methylolithium 27745-90-0 73635-95-7 73635-96-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P

652999-16-1P 652999-17-2P 652999-18-3P

652999-19-4P 652999-20-7P 652999-23-0P

652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P

652999-29-6P 652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P

653570-14-0P 653570-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 652999-15-0P 652999-21-8P 652999-22-9P 652999-28-5P

652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Chapman, O; US 5019660 A 1991 HCPLUS
- (2) Dahl, J; WO 02057201 A 2002 HCPLUS
- (3) Dahl, J; WO 02058139 A 2002 HCPLUS
- (4) Dahl, J; WO 03050066 A 2003 HCPLUS
- (5) Fritz, G; ANGEWANDTE CHEMIE, INTERNATIONAL EDITION IN ENGLISH 1970, V9(6), P464 HCPLUS
- (6) Fritz, G; ZEITSCHRIFT FUER ANORGANISCHE UND ALLGEMEINE CHEMIE 1984, V512, P103 HCPLUS
- (7) Marchand, A; SCIENCE 2003, V299(5603), P52 HCPLUS
- (8) Mobil Oil Corp; WO 9506019 A 1995 HCPLUS
- (9) Mochizuki, Y; CHEMICAL PHYSICS LETTERS 2001, V336(5,6), P451 HCPLUS

IT 652998-90-8, [121212121] Oxadecamantane  
 652998-91-9, [121212121] Thiadecamantane  
 652998-92-0, [121212121] Selenadecamantane  
 652998-93-1, [121212121] Boradecamantane  
 652998-94-2, [121212121] Azadecamantane  
 652998-95-3, [121212121] Phosphadecamantane  
 652998-96-4, [121212121] Arsadecamantane  
 652998-98-6, [1212121212] Oxaundecamantane  
 652998-99-7, [1212121212] Thiaundecamantane  
 652999-00-3, [1212121212] Selenaundercamantane  
 652999-01-4, [1212121212] Boraundecamantane  
 652999-02-5, [1212121212] Azaundecamantane  
 652999-03-6, [1212121212] Phosphaundecamantane  
 652999-04-7, [1212121212] Arsaundercamantane  
 652999-05-8 652999-06-9 652999-08-1  
 652999-09-2 652999-11-6 652999-12-7  
 652999-35-4 652999-36-5 652999-38-7  
 652999-39-8 652999-40-1, [121212121]  
 Boradecamantane 652999-41-2, [121212121]  
 Azadecamantane 652999-42-3, [121212121]  
 Phosphadecamantane 652999-43-4, [121212121]  
 Arsadecamantane 652999-44-5, [121212121]

**Boraundecamantane** 652999-45-6, [1212121212]

**Azaundecamantane** 652999-46-7, [1212121212]

**Phosphaundecamantane** 652999-47-8, [1212121212]

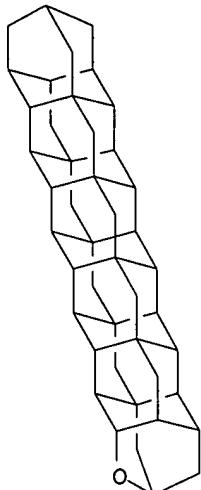
**Arsaundecamantane**

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids  
such as aza-, oxa-, and thiatetramantane from fused  
adamantanes such as tetramantanes)

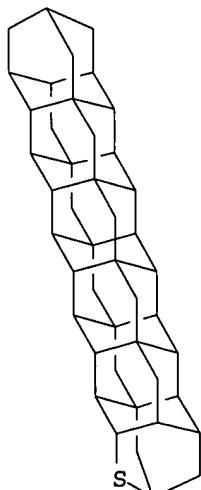
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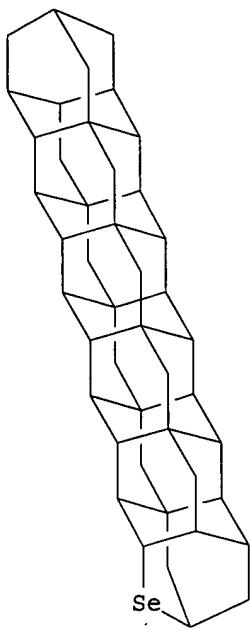
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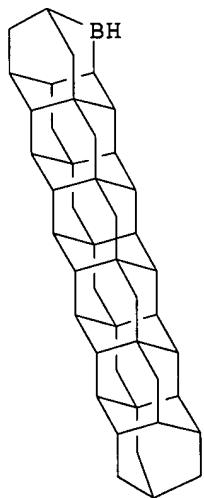


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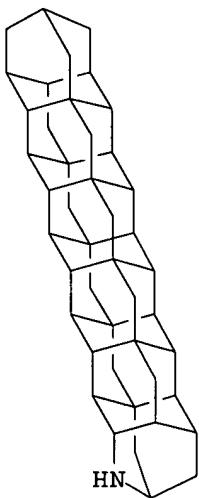
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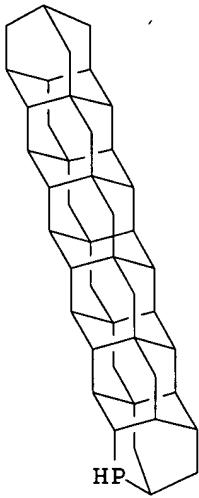
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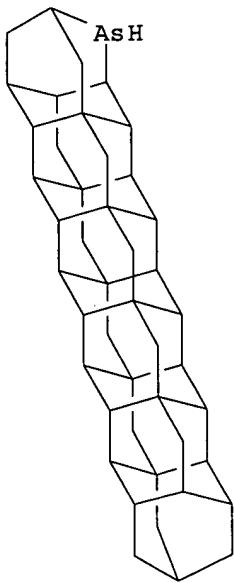
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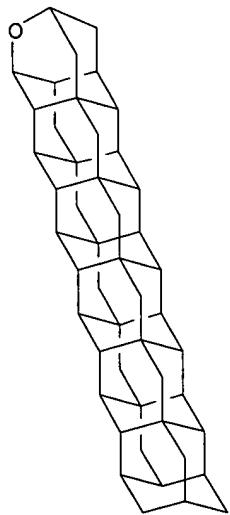
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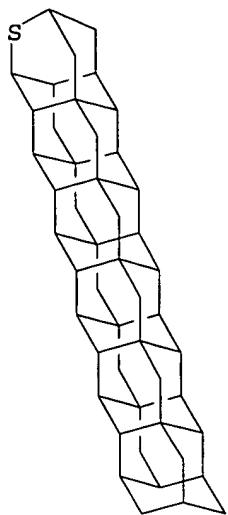
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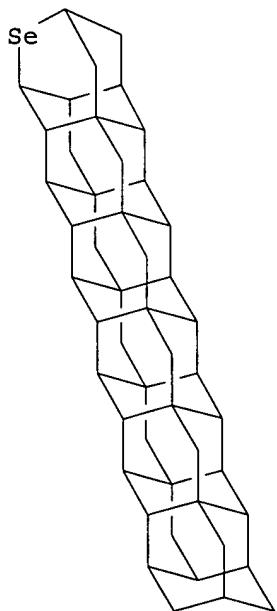
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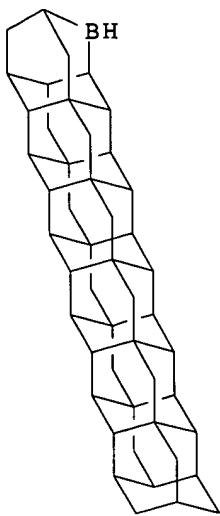
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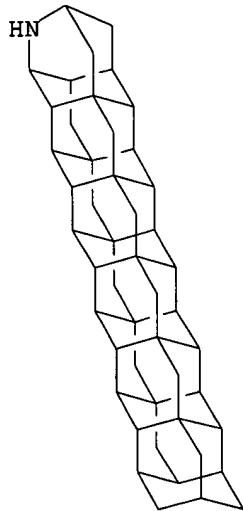
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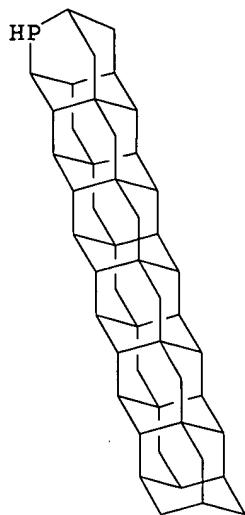
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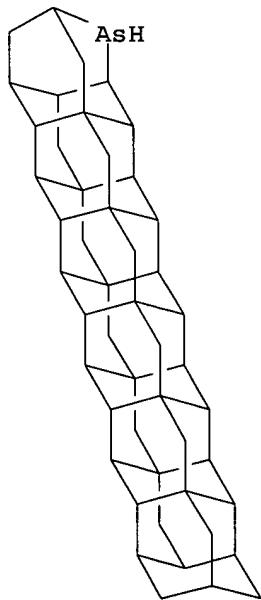
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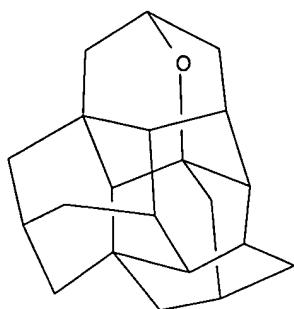
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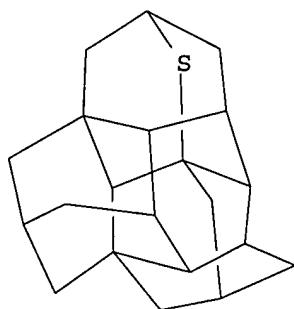


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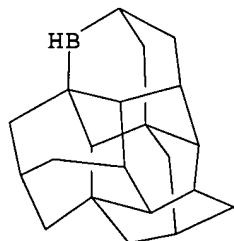
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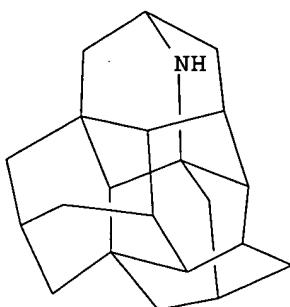
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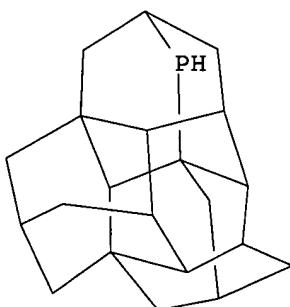
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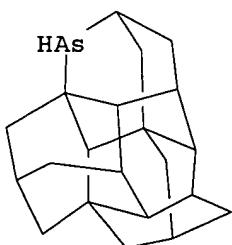
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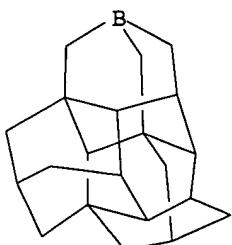
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CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphth[1,2,3-de]arsinoline, dodecahydro- (9CI) (CA INDEX NAME)



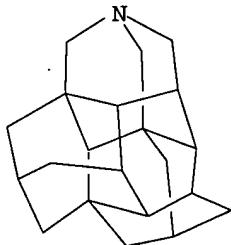
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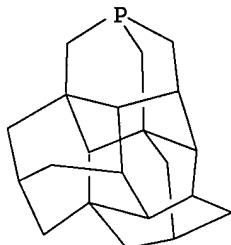
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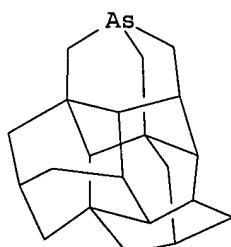
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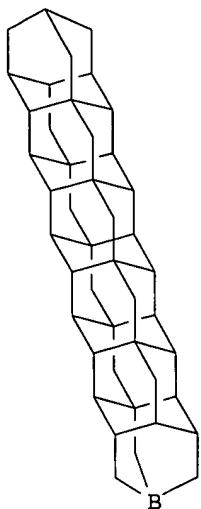
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CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoarsinoline, decahydro- (9CI) (CA INDEX NAME)

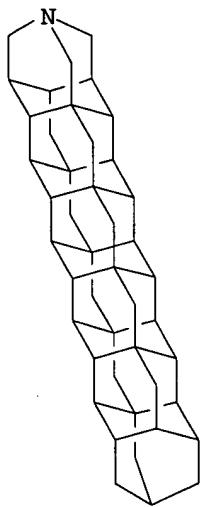


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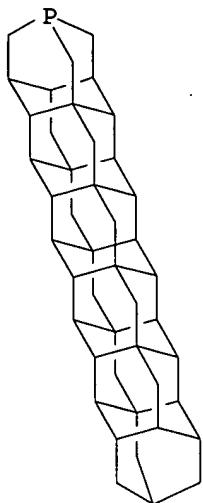
CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



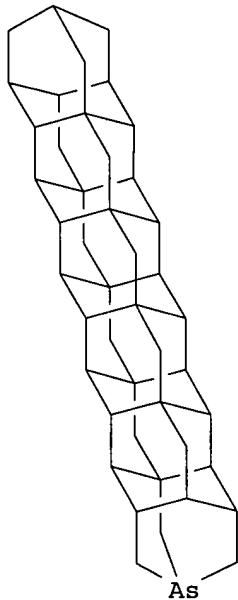
RN 652999-41-2 HCAPLUS  
CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



RN 652999-42-3 HCAPLUS  
CN [121212121] Phosphadecamantane (9CI) (CA INDEX NAME)

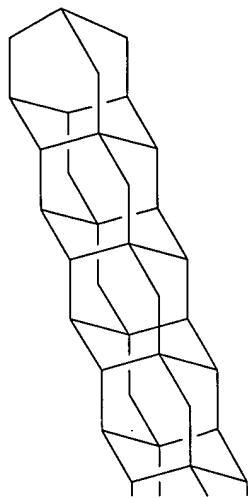


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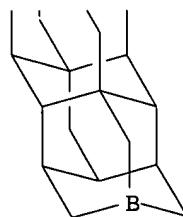


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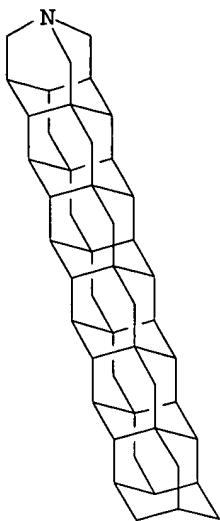
PAGE 1-A



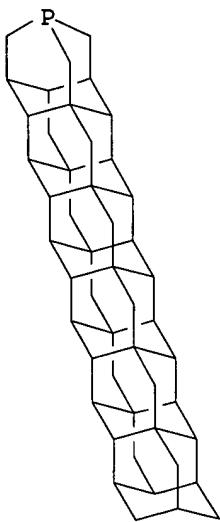
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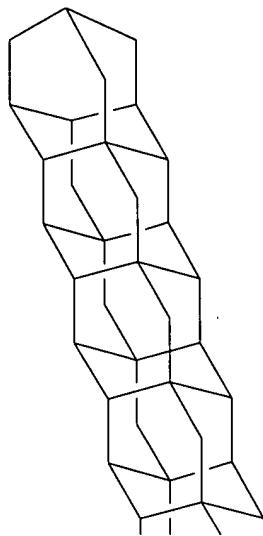


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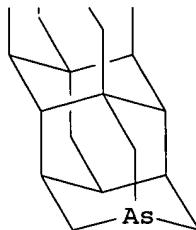


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PAGE 1-A



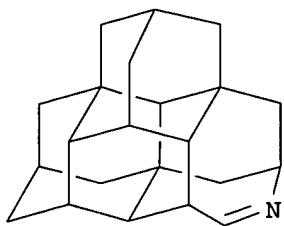
PAGE 2-A



IT    652999-16-1P 652999-17-2P 652999-18-3P  
      652999-19-4P 652999-20-7P 652999-23-0P  
      652999-24-1P 652999-25-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
      (preparation of heterodiamondoids such as aza-, oxa-, and  
      thiatetramantane from fused adamantanes such as  
      tetramantanes)

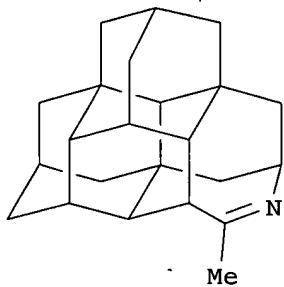
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      cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA  
      INDEX NAME)



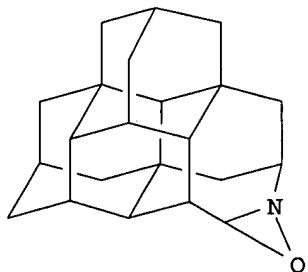
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(CA INDEX NAME)



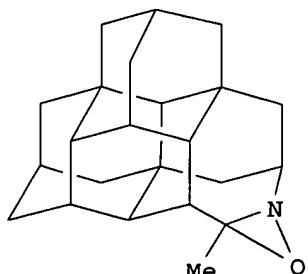
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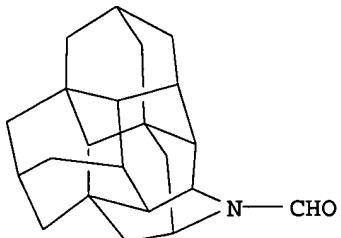
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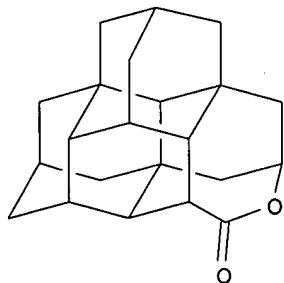
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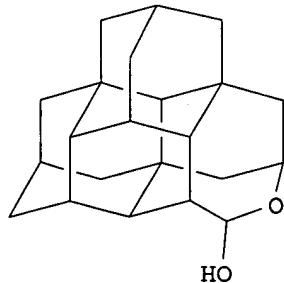
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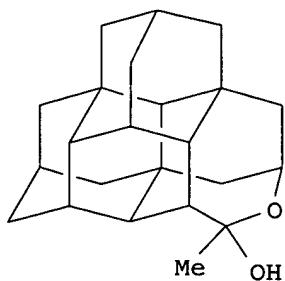
RN 652999-24-1 HCAPLUS

CN 5H, 8H-3, 12:6, 14-Dimethano-10, 8, 4a, 12-[1, 2]propanediyl[3]ylidene-1H-anthra[9, 1-cd]oxepin-1-ol, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-25-2 HCAPLUS

CN 5H, 8H-3, 12:6, 14-Dimethano-10, 8, 4a, 12-[1, 2]propanediyl[3]ylidene-1H-anthra[9, 1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)

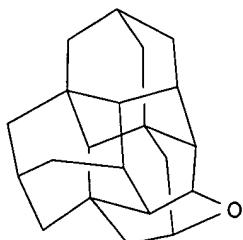


IT 652999-15-0P 652999-21-8P 652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of heterodiamondoids such as aza-, oxa-, and  
thiatetramantane from fused adamantanes such as  
tetramantanes)

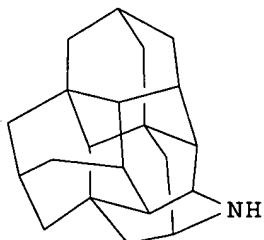
RN 652999-15-0 HCPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran, dodecahydro- (9CI) (CA INDEX NAME)



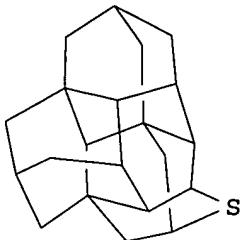
RN 652999-21-8 HCPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-32-1 HCPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



L64 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2003:800853 HCAPLUS  
 DN 140:339373  
 ED Entered STN: 13 Oct 2003  
 TI Theoretical analysis of a carbon-carbon dimer placement tool for diamond mechanosynthesis  
 AU Merkle, Ralph C.; Freitas, Robert A., Jr.  
 CS Zyvex Corp., Richardson, TX, USA  
 SO Journal of Nanoscience and Nanotechnology (2003), 3(4), 319-324  
 CODEN: JNNOAR; ISSN: 1533-4880  
 PB American Scientific Publishers  
 DT Journal  
 LA English  
 CC 29-6 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 22, 24  
 AB D. functional theory is used with Gaussian 98 to analyze a new family of proposed mechanosynthetic tools that could be employed for the placement of two carbon atoms-a carbon-carbon (CC) dimer-on a growing diamond surface at a specific site. Optimized structures and potential energies were calculated for 5,5'-ethynediyl-bridged 2,2',4,4',9,9'-biadamantane and its 5,5'-disila-, 5,5'-digerma-, 5,5'-distanna-, 5,5'-diplumba- and 5-sila-5-germa-analogs. The stationary points for the 5,5'-ethynediyl-, 5,5'-ethylidyne carbene and 2,2',4,4',5,5',9,9'-biadamantanes were located. The anal. focuses on specific Group IV-substituted biadamantane tool tip structures and evaluates their stability and the strength of the bond they make with the CC dimer. These tools should be stable in a vacuum and should be able to hold and position a CC dimer in a manner suitable for positionally controlled diamond mechanosynthesis at room temperature  
 ST biadamantane sila germa stanna plumba ethynediyl DFT geometry energy; carbon dimer placement tool biadamantane alkyne geometry potential energy; polycyclic compd condensed adamantane biadamantane heterocycle ethynediyl DFT calcn; heterocyclic compd silicon germanium tin lead polycyclic DFT energy; DFT geometry energy polycyclic adamantane Group IVA deriv calcn; diamond diamondoid hydrocarbon diadamantane hetero substituted DFT geometry energy; mol structure optimized hetero diadamantane ethynediyl linked  
 IT Density functional theory  
 (B3LYP; geometry optimization and potential energy of ethynediyl-linked heterobiadamantanes as carbon dimer precursors)  
 IT Potential energy  
 (DFT B3LYP geometry optimization and potential energy of ethynediyl-linked heterobiadamantanes as carbon dimer precursors)  
 IT Carbenes (methylene derivatives)  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (DFT B3LYP geometry optimization and potential energy of ethynediyl-linked heterobiadamantanes as carbon dimer

precursors)  
 IT Bond energy  
 (carbon-heteroatom bond energy of ethynediyl-linked  
**heterobiadamantanes** as carbon dimer precursors)  
 IT Dimers  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,  
 nonpreparative)  
 (carbon; DFT geometry optimization and potential energy of  
 ethynediyl-linked **heterobiadamantanes** as carbon dimer  
 precursors)  
 IT Hydrocarbons, properties  
 RL: PRP (Properties)  
 (**diamondoid, biadamantanes**; DFT B3LYP geometry  
 optimization and potential energy of ethynediyl-linked  
**heterobiadamantanes** as carbon dimer precursors)  
 IT Group IVA element compounds  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM  
 (Formation, nonpreparative); RACT (Reactant or reagent)  
 (**heterobiadamantanes**; DFT B3LYP geometry optimization and  
 potential energy of ethynediyl-linked **heterobiadamantanes** as  
 carbon dimer precursors)  
 IT Molecular structure  
 (optimized; of ethynediyl-linked **heterobiadamantanes** as  
 carbon dimer precursors)  
 IT Polycyclic compounds  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (tricyclic; DFT B3LYP geometry optimization and potential energy of  
 ethynediyl-linked **heterobiadamantanes** as carbon dimer  
 precursors)  
 IT 681029-73-2P 681029-74-3P 681029-75-4P  
 681029-76-5P 681029-77-6P  
 RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)  
 (DFT B3LYP geometry optimization and potential energy of  
 ethynediyl-linked **heterobiadamantanes** as carbon dimer  
 precursors)  
 IT 681029-78-7, [4,6]Fulleroid-C20 681029-79-8,  
 Disila[4,6]fulleroid-C20 681029-80-1, Digerma[4,6]fulleroid-C20  
 681029-81-2, Distanna[4,6]fulleroid-C20 681029-82-3,  
 Diplumba[4,6]fulleroid-C20 681029-83-4, Germasila[4,6]fulleroid-  
 C20  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,  
 nonpreparative)  
 (DFT B3LYP geometry optimization and potential energy of  
 ethynediyl-linked **heterobiadamantanes** as carbon dimer  
 precursors)  
 IT 681029-67-4 681029-68-5 681029-69-6  
 681029-70-9 681029-71-0 681029-72-1  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (fragmentation; DFT B3LYP geometry optimization and potential energy of  
 ethynediyl-linked **heterobiadamantanes** as carbon dimer  
 precursors)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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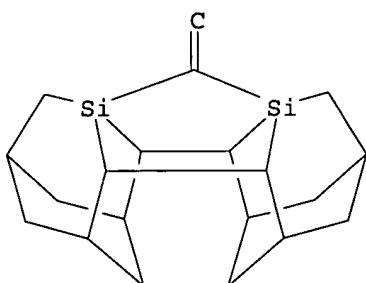
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**681029-77-6P**

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precursors)

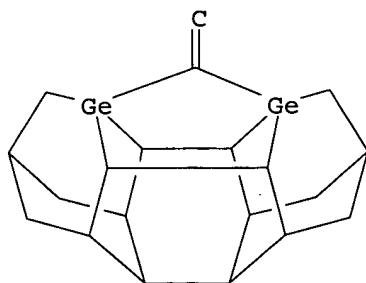
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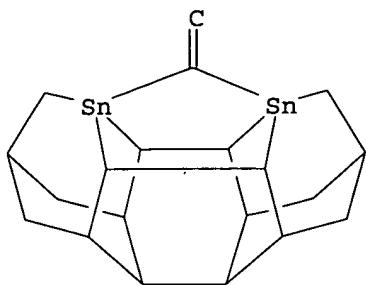
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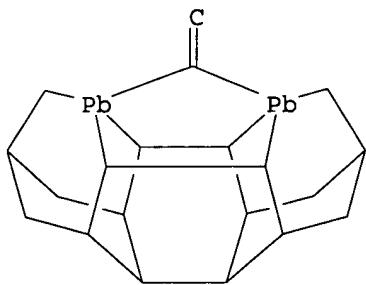


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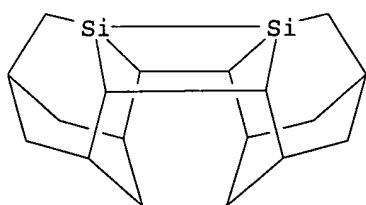


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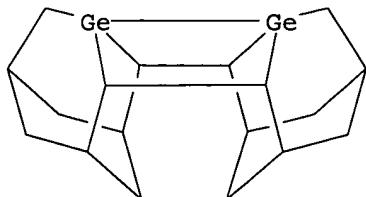


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 Digerma[4,6]fulleroid-C20 681029-81-2, Distanna[4,6]fulleroid-  
 C20 681029-82-3, Diplumba[4,6]fulleroid-C20 681029-83-4  
 , Germasila[4,6]fulleroid-C20  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,  
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 (DFT B3LYP geometry optimization and potential energy of  
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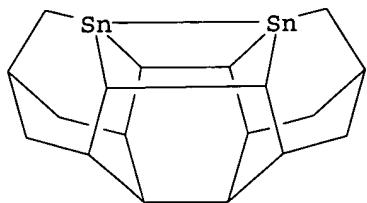
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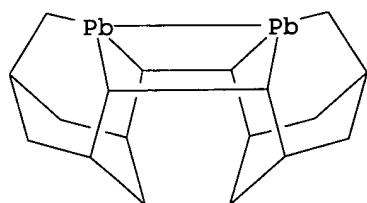
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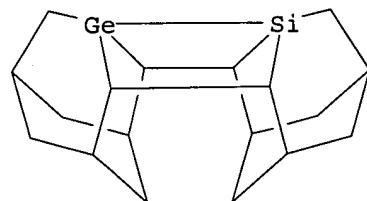
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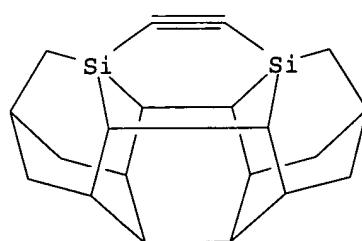


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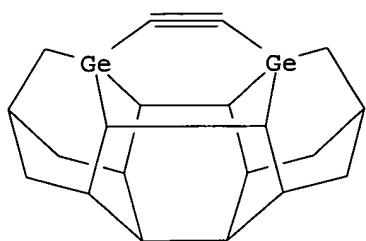


IT 681029-68-5 681029-69-6 681029-70-9  
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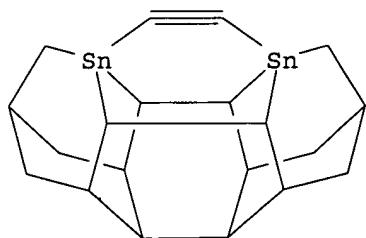
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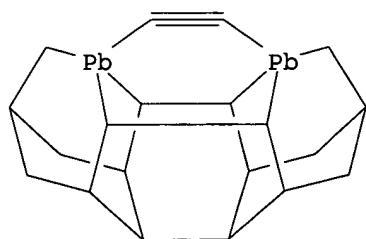
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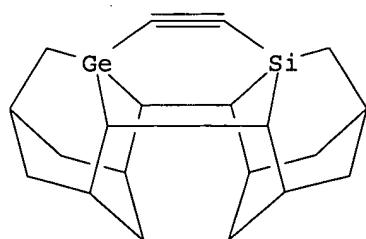
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RN 681029-71-0 HCPLUS  
CN Diplumba[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



RN 681029-72-1 HCPLUS  
CN Germasila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 10:24:18 ON 10 MAR 2005  
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STRUCTURE FILE UPDATES: 9 MAR 2005 HIGHEST RN 844817-50-1  
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

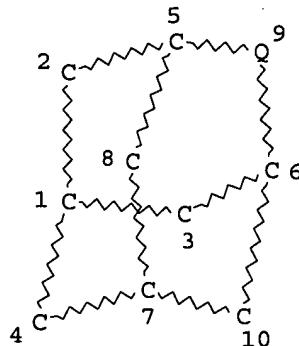
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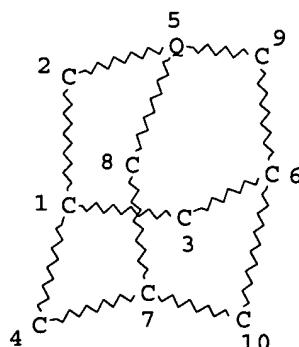
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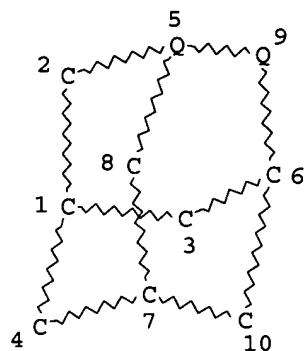
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 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
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STRUCTURE FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1  
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when

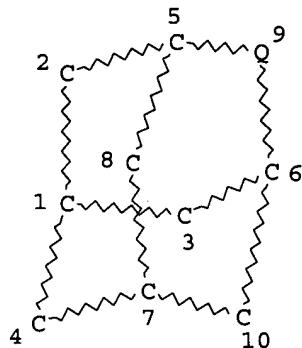
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Crossover limits have been increased. See HELP CROSSOVER for details.

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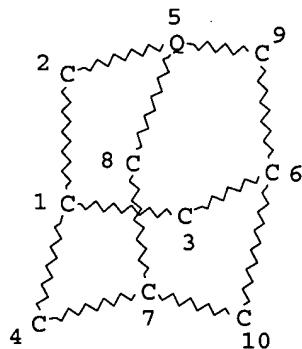
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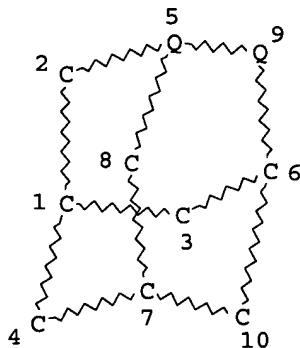
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STEREO ATTRIBUTES: NONE  
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## STEREO ATTRIBUTES: NONE

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L5 125 SEA FILE=REGISTRY SSS FUL (L1 OR L2 OR L3) AND L4

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125 ANSWERS

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ACT SHIAO622A/A

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L3      STR
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ACT SHIAO622/A
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L33 1 S L5 AND C21H24B2  
L34 16 S L31,L33  
SAV L34 SHIAO622B/A  
L35 9 S L29 NOT L32  
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L36 19 S E6-E29  
E 99573/RID  
L37 10 S E3-E13  
E 81072/RID  
L38 4 S E3-E8  
E 7965/RID  
L39 54 S E3-E56  
L40 25 S L39 NOT L29,L32,L34  
L41 7 S L40 AND (CU OR SI)/ELS  
L42 33 S L34,L37,L41  
L43 26 S L42 NOT L29  
L44 7 S L29 AND L42  
SAV L43 SHIAO622C/A

FILE 'HCAOLD' ENTERED AT 06:57:56 ON 14 MAR 2005

L45 0 S L29  
L46 0 S L43

FILE 'HCAPLUS' ENTERED AT 06:58:01 ON 14 MAR 2005

L47 8 S L43  
L48 1 S L47 AND (LIU S? OR CARLSON R? OR DAHL J?)/AU  
L49 1 S L47 AND CHEVRO?/PA,CS  
L50 1 S L48,L49  
L51 8 S L47,L50

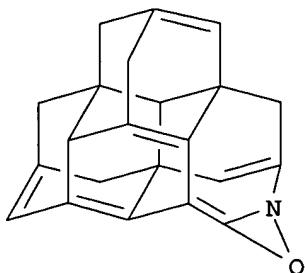
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L52 1 S L43

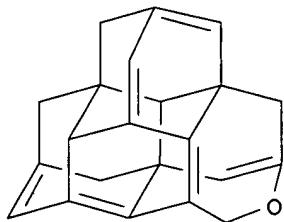
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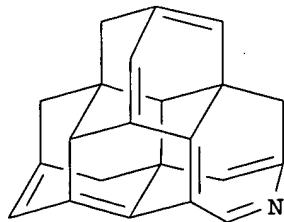
L43 ANSWER 1 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 656230-43-2 REGISTRY  
CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine (9CI) (CA INDEX NAME)  
MF C22 H15 N O  
CI RPS  
SR CA Index Guide or Ring Systems Handbook



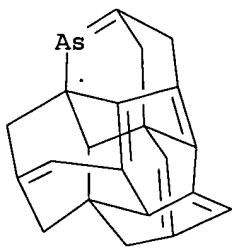
L43 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
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 MF C22 H16 O  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



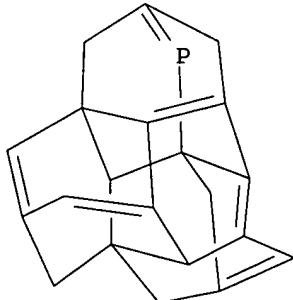
L43 ANSWER 3 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-40-9 REGISTRY  
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 MF C22 H15 N  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



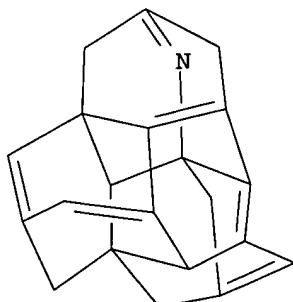
L43 ANSWER 4 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-39-6 REGISTRY  
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 MF C21 H15 As  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-38-5 REGISTRY  
 CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphtho[1,2,3-de]phosphinoline (9CI) (CA INDEX NAME)  
 MF C21 H15 P  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



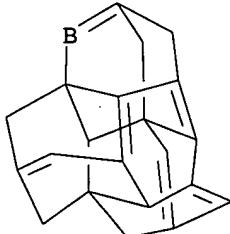
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 RN 656230-37-4 REGISTRY  
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 MF C21 H15 N  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



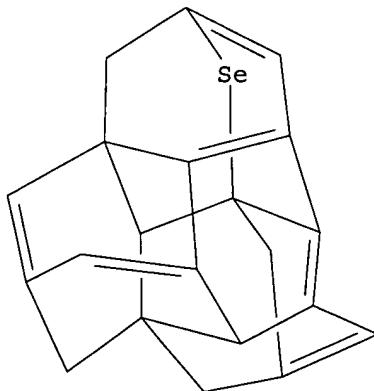
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L43 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-36-3 REGISTRY

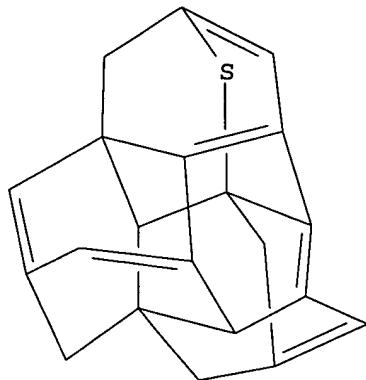
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 MF C21 H15 B  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-35-2 REGISTRY  
 CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin (9CI) (CA INDEX NAME)  
 MF C21 H14 Se  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook

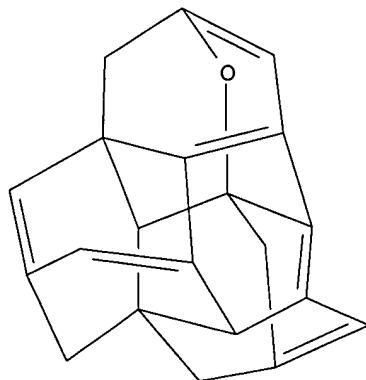


L43 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-34-1 REGISTRY  
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 MF C21 H14 S  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



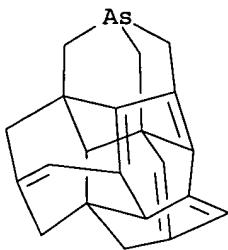
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L43 ANSWER 10 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 656230-33-0 REGISTRY  
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CI RPS  
SR CA Index Guide or Ring Systems Handbook

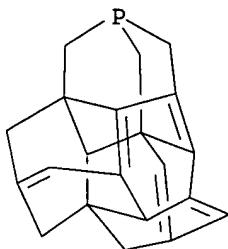


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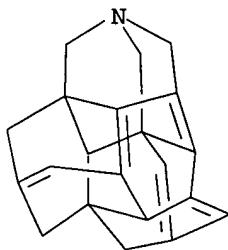
L43 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 656230-32-9 REGISTRY  
CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isoarsinoline (9CI) (CA INDEX NAME)  
MF C21 H17 As  
CI RPS  
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-31-8 REGISTRY  
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 MF C21 H17 P  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



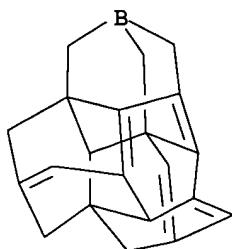
L43 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-30-7 REGISTRY  
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 MF C21 H17 N  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



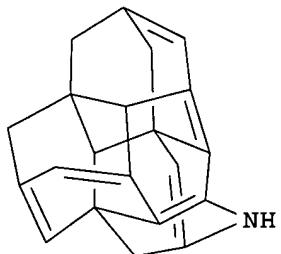
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L43 ANSWER 14 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
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 MF C21 H17 B

CI RPS  
 SR CA Index Guide or Ring Systems Handbook

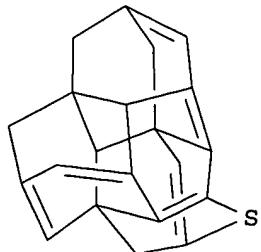


L43 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-28-3 REGISTRY  
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 MF C21 H15 N  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



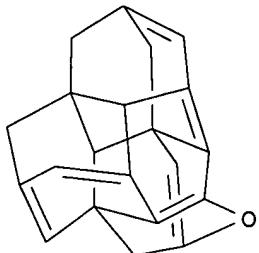
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 RN 656230-27-2 REGISTRY  
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 MF C21 H14 S  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



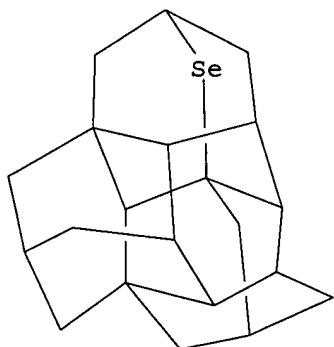
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L43 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 656230-26-1 REGISTRY  
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 MF C21 H14 O  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L43 ANSWER 18 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 652999-07-0 REGISTRY  
 CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-b]selenin, dodecahydro- (9CI) (CA INDEX NAME)  
 MF C21 H26 Se  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA CAplus document type: Patent  
 RL.P Roles from patents: PRP (Properties)



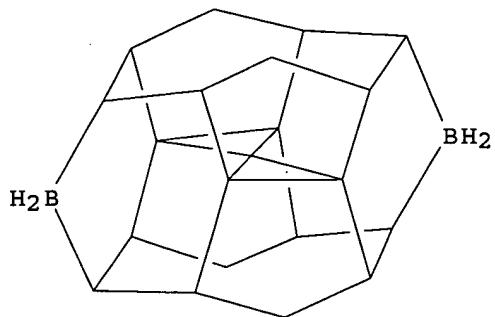
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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:146009

L43 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 475276-89-2 REGISTRY  
 CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-tetraseco[5]fullerane-C20-Ih, 21,23-dihydro- (9CI) (CA INDEX NAME)

MF C21 H24 B2  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RL.NP Roles from non-patents: PRP (Properties)



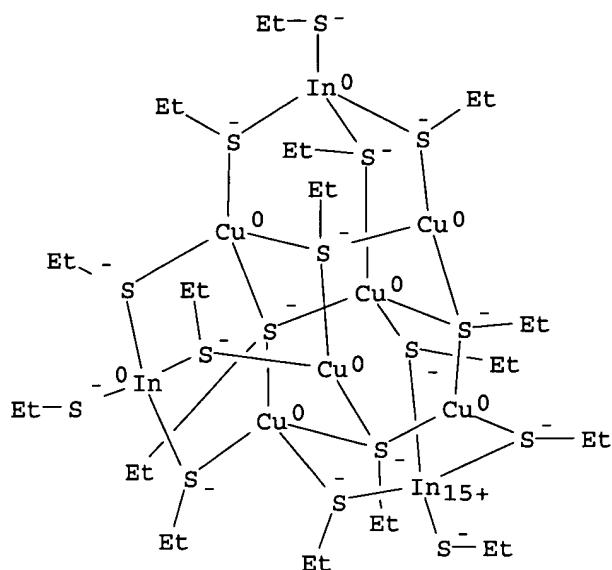
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REFERENCE 1: 137:370137

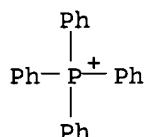
L43 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 142381-39-3 REGISTRY  
 CN Phosphonium, tetraphenyl-, nonakis[ $\mu$ -(ethanethiolato)]tetrakis[ $\mu$ 3-(ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Cuprate(1-), nonakis[ $\mu$ -(ethanethiolato)]tetrakis[ $\mu$ 3-(ethanethiolato)]tris[(ethanethiolato)indate]hexa-, tetraphenylphosphonium (9CI)  
 MF C32 H80 Cu6 In3 S16 . C24 H20 P  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

CM 1

CRN 142381-38-2  
 CMF C32 H80 Cu6 In3 S16  
 CCI CCS

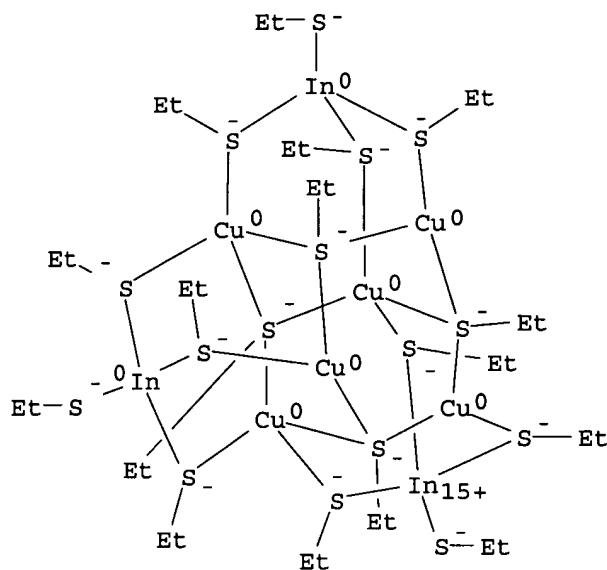


CM 2

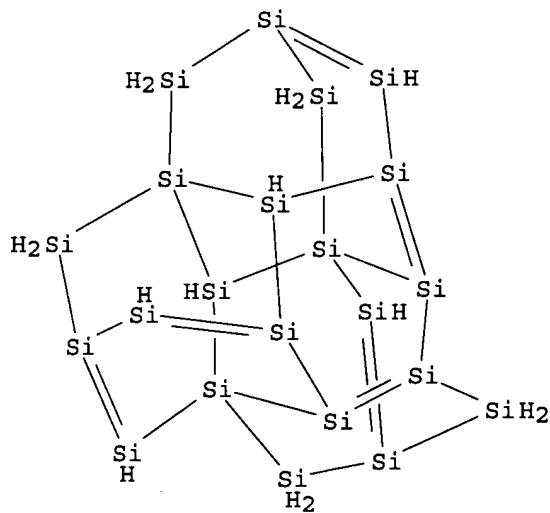
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REFERENCE 1: 117:61532

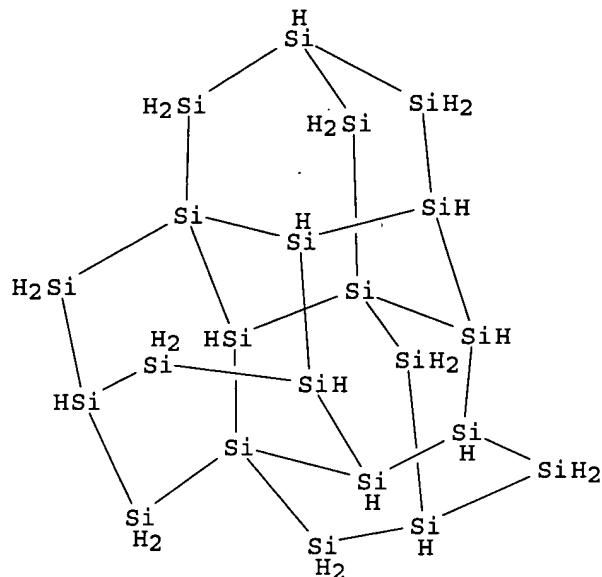
L43 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 142381-38-2 REGISTRY  
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 MF C32 H80 Cu6 In3 S16  
 CI CCS, COM  
 SR CA



L43 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 121472-96-6 REGISTRY  
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 MF H16 Si22  
 CI RPS  
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 119052-10-7 REGISTRY  
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 MF H28 Si22  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPplus document type: Journal  
 RL.NP Roles from non-patents: PRP (Properties)



3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:173087

REFERENCE 2: 135:10213

REFERENCE 3: 110:86206

L43 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN

RN 94396-97-1 REGISTRY

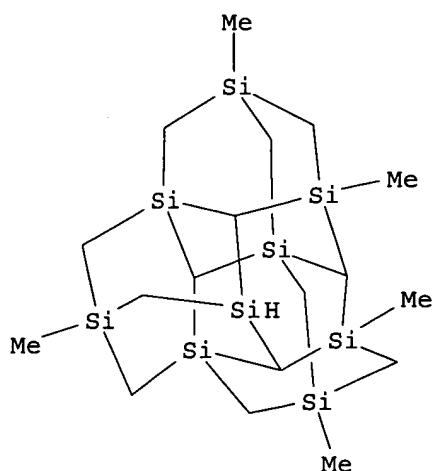
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9-pentamethyl- (9CI) (CA INDEX NAME)

MF C18 H38 Si9

LC STN Files: CA, CAPLUS

DT.CA CAPplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

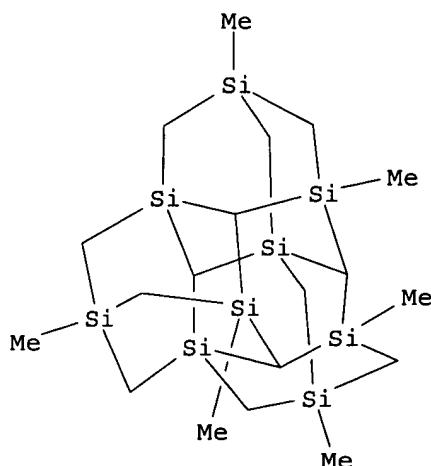


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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:78938

L43 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 31714-54-2 REGISTRY  
 CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-  
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-  
 2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)  
 MF C19 H40 Si9  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS  
 (\*File contains numerically searchable property data)  
 DT.CA Cplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation)



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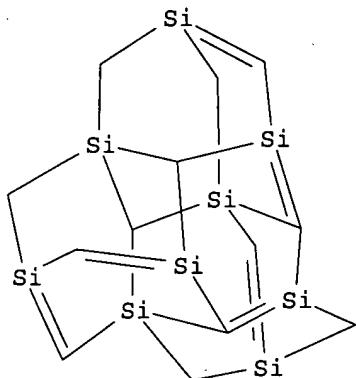
2 REFERENCES IN FILE CA (1907 TO DATE)

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REFERENCE 1: 102:78938

REFERENCE 2: 73:56178

L43 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 29861-92-5 REGISTRY  
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     2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene (9CI) (CA INDEX NAME)  
 MF C13 H16 Si9  
 CI RPS



=&gt; fil uspatful

FILE 'USPATFULL' ENTERED AT 07:01:15 ON 14 MAR 2005  
 CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Mar 2005 (20050310/PD)  
 FILE LAST UPDATED: 10 Mar 2005 (20050310/ED)  
 HIGHEST GRANTED PATENT NUMBER: US6865747  
 HIGHEST APPLICATION PUBLICATION NUMBER: US2005055750  
 CA INDEXING IS CURRENT THROUGH 10 Mar 2005 (20050310/UPCA)  
 ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Mar 2005 (20050310/PD)  
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005  
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
 >>> original, i.e., the earliest published granted patents or <<<  
 >>> applications. USPAT2 contains full text of the latest US <<<  
 >>> publications, starting in 2001, for the inventions covered in <<<  
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 >>> published document but also a list of any subsequent <<<  
 >>> publications. The publication number, patent kind code, and <<<  
 >>> publication date for all the US publications for an invention <<<  
 >>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
 >>> records and may be searched in standard search fields, e.g., /PN, <<<  
 >>> /PK, etc. <<<

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 >>> through the new cluster USPATALL. Type FILE USPATALL to <<<  
 >>> enter this cluster. <<<  
 >>> <<<  
 >>> Use USPATALL when searching terms such as patent assignees, <<<  
 >>> classifications, or claims, that may potentially change from <<<

>>> the earliest to the latest publication.

<<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> => d bib abs hitstr 152

L52 ANSWER 1 OF 1 USPATFULL on STN  
AN 2004:77366 USPATFULL  
TI Heterodiamondoids  
IN Liu, Shenggao, Hercules, CA, UNITED STATES  
Carlson, Robert M., Petaluma, CA, UNITED STATES  
Dahl, Jeremy E., Palo Alto, CA, UNITED STATES  
PA CHEVRON USA INC. (U.S. corporation)  
PI US 2004059145 A1 20040325  
AI US 2003-622130 A1 20030716 (10)  
PRAI US 2002-397367P 20020718 (60)  
DT Utility  
FS APPLICATION  
LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404,  
Alexandria, VA, 22313-1404  
CLMN Number of Claims: 37  
ECL Exemplary Claim: 1  
DRWN 51 Drawing Page(s)  
LN.CNT 2469  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention is related to heteroatom containing diamondoids (i.e., "heterodiamondoids") which are compounds having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compounds carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices can serve as optically active materials.

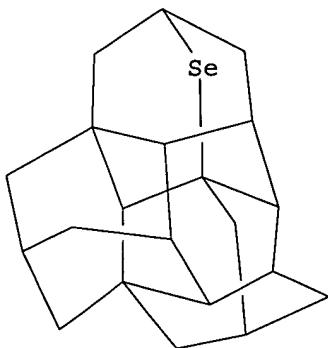
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 652999-07-0

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

RN 652999-07-0 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)



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FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L51 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:80675 HCAPLUS  
DN 140:146009  
ED Entered STN: 01 Feb 2004  
TI Preparation of heterodiamondoids from fused adamantanes  
IN Liu, Shenggao; Carlson, Robert M.  
PA Chevron U.S.A. Inc., USA; Dahl, Jeremy E.  
SO PCT Int. Appl., 134 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM C07D311-78  
ICS C07D313-06; C07D335-04; C07D221-18  
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 76  
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI WO 2004009577	A1	20040129	WO 2003-US22483	20030717

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,  
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,  
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004059145 A1 20040325 US 2003-622130 20030716

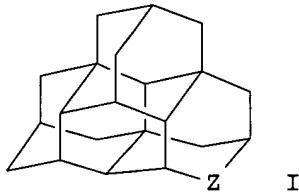
PRAI US 2002-397367P P 20020718  
 US 2002-397368P P 20020718

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
	ICS	C07D313-06; C07D335-04; C07D221-18
US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C

OS MARPAT 140:146009

GI



*SJF*

- AB This invention is related to heteroatom containing diamondoids (i.e., 'heterodiamondoids'), e.g. azatetramantane, oxatetramantane, and thiatetramantane (I; X = NH, O, S), which are compds. having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).
- ST heterodiamondoid prep; azatetramantane oxatetramantane thiatetramantane prep
- IT Formation enthalpy  
 (preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)
- IT Heterocyclic compounds  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)
- IT 652998-89-5, [121212121] Decamantane 652998-90-8, [121212121]  
 Oxadecamantane 652998-91-9, [121212121] Thiadecamantane 652998-92-0,  
 [121212121] Selenadecamantane 652998-93-1, [121212121] Boradecamantane  
 652998-94-2, [121212121] Azadecamantane 652998-95-3, [121212121]  
 Phosphadecamantane 652998-96-4, [121212121] Arsadecamantane

652998-97-5, [1212121212] Undecamantane 652998-98-6, [1212121212]  
 Oxaundecamantane 652998-99-7, [1212121212] Thiaundecamantane  
 652999-00-3, [1212121212] Selenaundecamantane 652999-01-4, [1212121212]  
 Boraundecamantane 652999-02-5, [1212121212] Azaundecamantane  
 652999-03-6, [1212121212] Phosphaundecamantane 652999-04-7, [1212121212]  
 Arsaundecamantane 652999-05-8 652999-06-9 **652999-07-0**  
 652999-08-1 652999-09-2 652999-11-6 652999-12-7 652999-35-4  
 652999-36-5 652999-38-7 652999-39-8 652999-40-1, [121212121]  
 Boradecamantane 652999-41-2, [121212121] Azadecamantane 652999-42-3,  
 [121212121] Phosphadecamantane 652999-43-4, [121212121] Arsadecamantane  
 652999-44-5, [1212121212] Boraundecamantane 652999-45-6, [1212121212]  
 Azaundecamantane 652999-46-7, [1212121212] Phosphaundecamantane  
 652999-47-8, [1212121212] Arsaundecamantane

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,  
 oxa-, and thiatetramantane from fused adamantanes such as  
 tetramantanes)

IT 917-54-4, Methylolithium 27745-90-0 73635-95-7 73635-96-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane  
 from fused adamantanes such as tetramantanes)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P 652999-16-1P

652999-17-2P 652999-18-3P 652999-19-4P 652999-20-7P 652999-23-0P

652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P 652999-29-6P

652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P 653570-14-0P

653570-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane  
 from fused adamantanes such as tetramantanes)

IT 652999-15-0P 652999-21-8P 652999-22-9P 652999-28-5P 652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane  
 from fused adamantanes such as tetramantanes)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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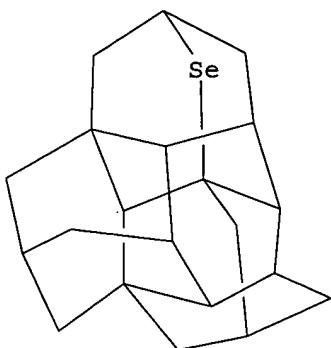
IT **652999-07-0**

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,  
 oxa-, and thiatetramantane from fused adamantanes such as  
 tetramantanes)

RN 652999-07-0 HCPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2002:685440 HCAPLUS  
 DN 137:370137  
 ED Entered STN: 11 Sep 2002  
 TI The Theoretical Design of Neutral Planar Tetracoordinate Carbon Molecules  
 with C(C)4 Substructures  
 AU Wang, Zhi-Xiang; Schleyer, Paul von Rague  
 CS Computational Chemistry Annex, University of Georgia, Athens, GA,  
 30602-2525, USA  
 SO Journal of the American Chemical Society (2002), 124(40), 11979-11982  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 29-4 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 22, 24  
 AB Using a new charge-compensation strategy, neutral mols. were designed with perfectly planar C(C)4-type tetracoordinate carbon arrangements (ptC) employing DFT computations. These designs, based on the planar preference of methane dications, replace two remote carbons in spiroalkaplanes by borons or two remote hydrogens by BH<sub>3</sub> groups; the two formally anionic boron units which result compensate the formal double pos. charge on the central ptC's. The LUMOs correspond to the "wasted" lone pair HOMOs of the alkaplanes. As compared to the latter,  $\pi$  occupancies on the central carbon are much smaller (less than 0.7e), and the IPs are much larger. The newly predicted compds. utilize all of the electrons more effectively. There are no lone pairs, and the ptC-C bond lengths are ca. 1.50 Å. The Wiberg bond index sums of the ptC's are near 3.2, and the boron sums are close to 4.  
 ST planar tetracoordinate carbon boron compd DFT; mol electronic structure  
 spiroalkaplane boron compd DFT; HOMO planar tetracoordinate carbon boron  
 compd DFT  
 IT Molecular structure  
     (optimized; theor. study of tetracoordinate carbon mols. with C(C)4  
     substructures)  
 IT Stereochemistry  
     (tetrahedral vs. planar; theor. study of tetracoordinate carbon mols.  
     with C(C)4 substructures)  
 IT Density functional theory  
 Electronic structure  
 HOMO (molecular orbital)  
 Stabilization energy  
     (theor. study of tetracoordinate carbon mols. with C(C)4 substructures)  
 IT 74-82-8, Methane, properties 157-40-4, Spiropentane 20741-88-2,  
 Methane(1+), properties 73353-64-7, Indeno[7,1-cd]indene 101517-28-6,  
 Spiro[2.2]pentane, radical ion(1+) 148810-14-4, Methane, radical

ion(2+), properties 179032-57-6, Spiro[2.2]octaplane 251918-68-0  
 330597-93-8 475276-87-0 475276-88-1 **475276-89-2**  
 475276-90-5 475276-91-6 475276-92-7 475276-93-8 475276-94-9  
 475276-95-0 475276-96-1 475276-97-2 475276-98-3 475467-16-4  
 475467-22-2

RL: PRP (Properties)

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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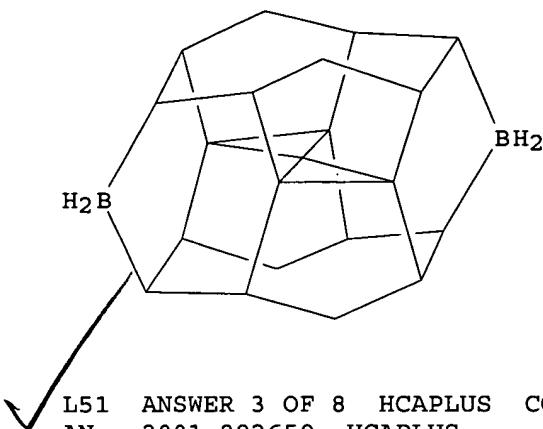
IT **475276-89-2**

RL: PRP (Properties)

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RN 475276-89-2 HCPLUS

CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-tetraseco[5]fullerane-C20-Ih, 21,23-dihydro- (9CI) (CA INDEX NAME)



L51 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2001:892659 HCAPLUS  
 DN 136:173087  
 ED Entered STN: 12 Dec 2001  
 TI Size, Order, and Dimensional Relations for Silicon Cluster  
 Polarizabilities  
 AU Jansik, B.; Schimmelpfennig, B.; Norman, P.; Mochizuki, Y.; Luo, Y.;  
 Aagren, H.  
 CS Theoretical Chemistry, Royal Institute of Technology, Stockholm, S-106 91,  
 Swed.  
 SO Journal of Physical Chemistry A (2002), 106(2), 395-399  
 CODEN: JPCAFH; ISSN: 1089-5639  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 65-5 (General Physical Chemistry)  
 AB Response theory calcns. in the RPA are applied to linear polarizabilities  
 and second hyperpolarizabilities of 1-, 2-, and 3-dimensional  
 hydrogen-terminated silicon clusters. Successive enlargement of the  
 clusters to embody on the order of 50 silicon atoms plus bond-saturating  
 hydrogen atoms allows for extrapolation to bulk values of individual  
 silicon atom contributions in the 1D and 3D cases. Modern effective core  
 potentials are shown to provide excellent approxns. to the all-electron  
 values in all cases; errors for both polarizabilities and  
 hyperpolarizabilities are on the order of 1%. The findings indicate  
 considerable time savings in predictions of the elec. polarizability  
 properties of elements beyond the first row atoms.  
 ST silicon cluster hydrogen termination polarizability hyperpolarizability  
 response theory RPA; effective core potential silicon cluster hydrogen  
 termination polarizability hyperpolarizability  
 IT Basis sets  
     (effectiveness core potential; in study of polarizabilities and  
     hyperpolarizabilities of hydrogen-terminated silicon clusters with  
     size, order, and dimensional relations studied by response theory in  
     RPA)  
 IT Electron correlation  
     (in study of polarizabilities and hyperpolarizabilities of  
     hydrogen-terminated silicon clusters with size, order, and dimensional  
     relations studied by response theory in RPA)  
 IT Cluster structure  
 Hyperpolarizability  
 Polarizability  
     (of hydrogen-terminated silicon clusters with size, order, and  
     dimensional relations studied by response theory in RPA)  
 IT Clusters  
 Size effect  
     (polarizabilities and hyperpolarizabilities of hydrogen-terminated  
     silicon clusters with size, order, and dimensional relations studied by

response theory in RPA)

IT Silanes

RL: PRP (Properties)

(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

IT 291-59-8, Cyclohexasilane 1590-87-0, Silicon hydride (Si<sub>2</sub>H<sub>6</sub>)  
 7783-26-8, Silicon hydride (Si<sub>3</sub>H<sub>8</sub>) 7783-29-1, Silicon hydride (Si<sub>4</sub>H<sub>10</sub>)  
 14693-61-9, Hexasilane 39517-09-4, Octasilane 41518-75-6, Decasilane  
 72244-91-8, Tetradecasilane 94570-81-7, Triacontasilane 99759-72-5,  
 Hexasilabenzene 119052-10-7 128171-51-7, Eicosasilane  
 133754-37-7, Hexadecasilane 153549-12-3, Pentadecasilane 155101-73-8,  
 Tricyclo[3.3.1.1.3,7]decasilane 209683-92-1, Dodecasilane 226714-57-4  
 334939-73-0, Silicon hydride (Si<sub>35</sub>H<sub>36</sub>) 340809-92-9 397250-81-6,  
 Dopentaccontasilane 397250-82-7, Hexadecasilapryrene 397250-83-8,  
 Tetracosasilacoronene 397250-84-9 397250-85-0, Silicon hydride  
 (Si<sub>54</sub>H<sub>56</sub>)

RL: PRP (Properties)

(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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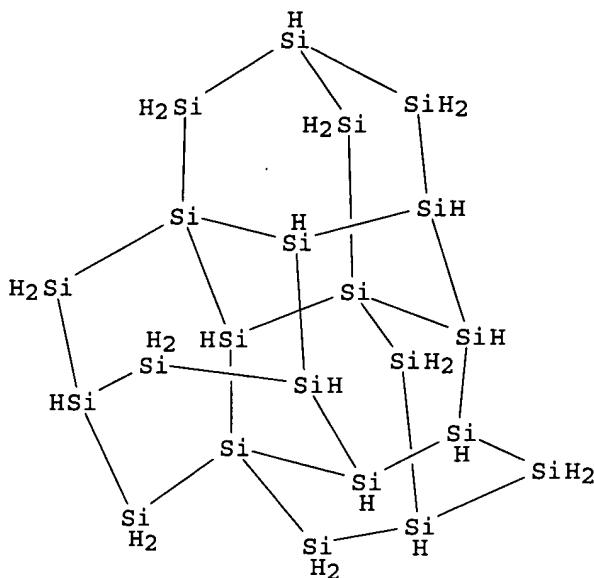
IT 119052-10-7

RL: PRP (Properties)

(polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

RN 119052-10-7 HCPLUS

CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



✓ L51 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2001:207328 HCAPLUS  
 DN 135:10213  
 ED Entered STN: 22 Mar 2001  
 TI Polarizability of silicon clusters  
 AU Mochizuki, Y.; Agren, H.  
 CS CCSE, Japan Atomic Energy Research Institute, Meguro-ku, Tokyo, 153-0061, Japan  
 SO Chemical Physics Letters (2001), 336(5,6), 451-456  
 CODEN: CHPLBC; ISSN: 0009-2614  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 CC 65-5 (General Physical Chemistry)  
 Section cross-reference(s): 76  
 AB The polarizability of hydrogen-terminated silicon clusters derived from the silicon diamond-lattice structure was evaluated by linear response calcns. The dependences on cluster size and basis set were systematically investigated. A convergence in calculated polarizability per silicon atom toward the bulk value was found. Frequency-dependent polarizabilities were also addressed.  
 ST polarizability silicon cluster  
 IT Cluster structure  
 Polarizability  
 (polarizability of silicon clusters)  
 IT 291-59-8, Cyclohexasilane 7440-21-3, Silicon, properties  
**119052-10-7** 147207-30-5, Silicon hydride (Si<sub>35</sub>H<sub>36</sub>)  
 212783-55-6, Silicon hydride (Si<sub>5</sub>H) 226714-57-4 312613-06-2, Silicon hydride (Si<sub>10</sub>H<sub>16</sub>) 340809-92-9  
 RL: PRP (Properties)  
 (polarizability of silicon clusters)  
 RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Anon; CRC Handbook of Chemistry and Physics, 79th ed 1998-1999  
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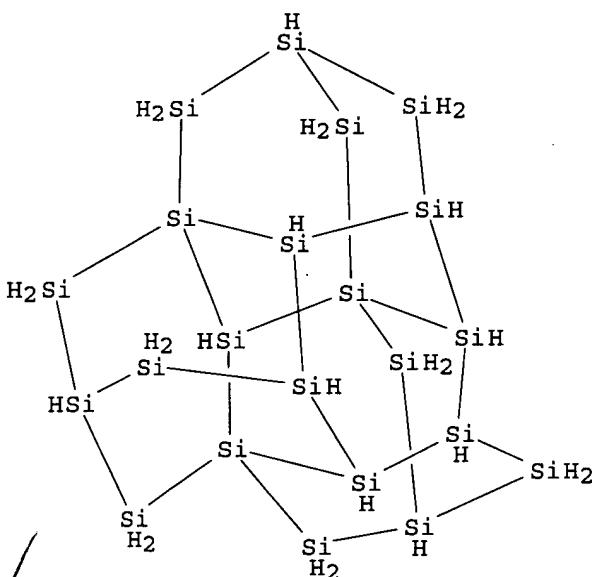
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IT 119052-10-7

RL: PRP (Properties)  
(polarizability of silicon clusters)

RN 119052-10-7 HCAPLUS

CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)

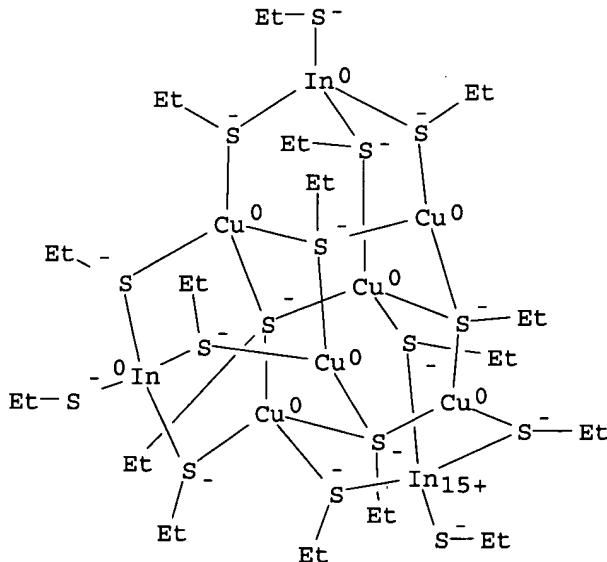


- L51 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1992:461532 HCAPLUS  
 DN 117:61532  
 ED Entered STN: 08 Aug 1992  
 TI Synthesis and structure of the first indium-copper cluster,  
 $[Cu_6In_3(SET)_{16}]^-$  and its possible relevance to CuInS<sub>2</sub>  
 AU Hirpo, Wakgari; Dhingra, Sandeep; Kanatzidis, Mercouri G.  
 CS Cent. Fundam. Mater. Res., Michigan State Univ., East Lansing, MI, 48824,  
 USA  
 SO Journal of the Chemical Society, Chemical Communications (1992), (7),  
 557-9  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DT Journal  
 LA English

CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 75  
 AB ( $\text{Ph}_4\text{P}^-$ )  $[\text{Cu}_6\text{In}_3(\text{SEt})_{16}]$  was prepared by the reaction of  $[\text{Cu}(\text{MeCN})_4]\text{PF}_6$  with  $(\text{Ph}_4\text{P}^-)[\text{In}(\text{SEt})_4]$  and its crystal structure shows an adamantoid framework.  
 ST crystal structure copper indium ethanethiolato cluster; thiolato copper indium nonanuclear cluster  
 IT Crystal structure  
 Molecular structure  
 (of copper indium ethanethiolato nonanuclear cluster)  
 IT Cluster compounds, coordinative  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (copper-indium-sulfur, ethanethiolato, preparation and crystal structure of)  
 IT 142381-39-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 IT 142029-65-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with copper acetonitrile complex)  
 IT 64443-05-6, Tetrakis(acetonitrile)copper(1+) hexafluorophosphate(1-)  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with indate ethanethiolato complex)  
 IT 142381-39-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 142381-39-3 HCPLUS  
 CN Phosphonium, tetraphenyl-, nonakis[ $\mu$ -(ethanethiolato)]tetrakis[ $\mu$ 3-(ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA INDEX NAME)

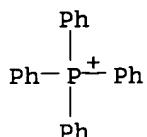
CM 1

CRN 142381-38-2  
 CMF C32 H80 Cu6 In3 S16  
 CCI CCS

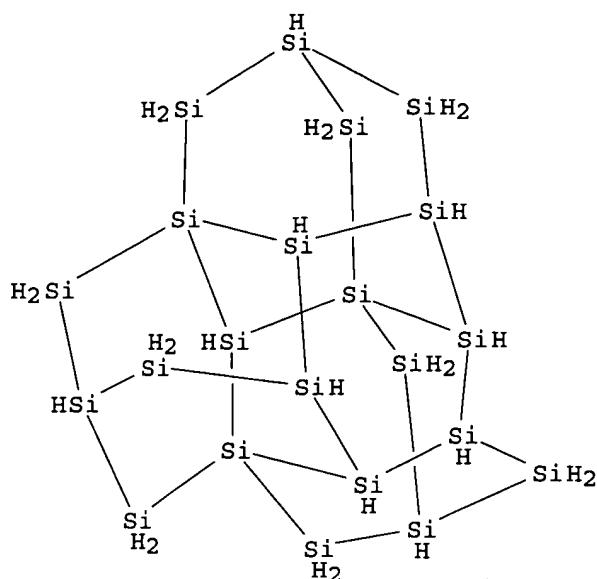


CM 2

CRN 18198-39-5  
 CMF C24 H20 P



LS1 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1989:86206 HCAPLUS  
 DN 110:86206  
 ED Entered STN: 04 Mar 1989  
 TI Hyperfine interactions in cluster models of the Pb defect center  
 AU Cook, Michael; White, C. T.  
 CS Nav. Res. Lab., Washington, DC, 20375-5000, USA  
 SO Physical Review B: Condensed Matter and Materials Physics (1988), 38(14),  
 9674-85  
 CODEN: PRBMDO; ISSN: 0163-1829  
 DT Journal  
 LA English  
 CC 76-1 (Electric Phenomena)  
 AB Hyperfine interactions in the Pb center (denoted schematically as Si3.tplbond.Si.), an electron trap, at the Si(111)/SiO<sub>2</sub> interface have been studied with use of spin-polarized self-consistent multiple-scattering X<sub>a</sub> calcns. on Si<sub>22</sub>H<sub>21</sub>/Si<sub>6</sub>O<sub>18</sub>H<sub>6</sub> and Si<sub>22</sub>H<sub>27</sub> cluster models. The theor. hyperfine tensor agrees very well with experiment when the trivalent atom Si' is relaxed by a value typical of geometries found for the neutral paramagnetic charge state in semiempirical and ab initio cluster calcns. Spin-polarization effects are very important for a detailed description of the Pb defect, particularly with respect to the hyperfine couplings at nuclei close to the defect atom. The largest such superhyperfine interaction is produced not by the nearest-neighbor atoms as has commonly been assumed, but by 3 second-nearest neighbors located below Si' in the bulk c-Si. The isotropic and anisotropic superhyperfine components and the direction of the principle axes predicted by the present calcns. have been confirmed by recent ESR expts.  
 ST interface silicon silica hyperfine interaction center  
 IT Trapping and Traps  
     (at silicon interface with silicon, cluster model of center for)  
 IT Interface  
     (silica-silicon, Pb center hyperfine interaction at, spin-polarized self-consistent multiple-scattering X<sub>a</sub> calcn. on)  
 IT 7440-21-3, Silicon, properties  
 RL: PRP (Properties)  
     (defect center hyperfine interaction at interface of silica with)  
 IT 7631-86-9, Silica, properties  
 RL: PRP (Properties)  
     (defect center hyperfine interaction at interface of silicon with)  
 IT 119052-09-4 119052-10-7  
 RL: PRP (Properties)  
     (interface defect center hyperfine interaction at silicon-silica interface from cluster model of)  
 IT 119052-10-7  
 RL: PRP (Properties)  
     (interface defect center hyperfine interaction at silicon-silica interface from cluster model of)  
 RN 119052-10-7 HCAPLUS  
 CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediyl[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 1985:78938 HCPLUS  
 DN 102:78938  
 ED Entered STN: 09 Mar 1985  
 TI Formation of organosilicon compounds. 100. Isolation of higher molecular weight carbosilanes from the pyrolysis of tetramethylsilane  
 AU Fritz, G.; Woerns, K. P.  
 CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, D-7500, Fed. Rep. Ger.  
 SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1984), 512, 103-25  
 CODEN: ZAACAB; ISSN: 0044-2313  
 DT Journal  
 LA German  
 CC 29-6 (Organometallic and Organometalloidal Compounds)  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A systematic investigation of the carbosilanes containing 6 to 9 Si atoms per mol. formed by pyrolysis of SiMe<sub>4</sub> was achieved by means of column chromatog. sepns. combined with HPLC. Eleven pure compds. and mixts. of I (R = Me, R<sub>1</sub> = CH<sub>2</sub>SiMe<sub>2</sub>CH<sub>2</sub>SiMe<sub>3</sub>; R = R<sub>1</sub> = Me<sub>3</sub>SiCH<sub>2</sub>) as well as of II and III were isolated. The predominant structure is that of the carborundanes using only Me and H as Si substituents. Only in compds. IV and V are some of the Si-C 6-membered rings in the chair form. In compds. such as VI another possibility of connecting 1,3,5,7-tetrasilaadamantane frameworks to higher mol. carbosilanes is realized.  
 ST silane tetramethyl pyrolysis; pyrolysis methylsilane; polycyclic carbosilane; silane silaadamantane poly  
 IT Chromatography, column and liquid  
     (high-performance, isolation of high mol. weight carbosilanes from the pyrolysis of tetramethylsilane by)  
 IT 26393-20-4P 31714-54-2P 94396-94-8P 94396-95-9P  
 94396-96-0P 94396-97-1P 94396-98-2P 94396-99-3P  
 94397-00-9P  
 RL: PREP (Preparation)  
     (isolation of, from pyrolysis of tetramethylsilane)

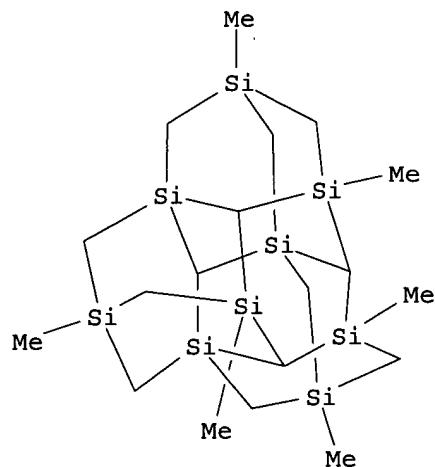
IT 50938-70-0P 65000-98-8P 86932-03-8P 94396-90-4P 94396-91-5P  
 94396-92-6P 94396-93-7P 94411-13-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by pyrolysis of tetramethylsilane)

IT 75-76-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (pyrolysis of, isolation of higher mol. weight carbosilanes from)

IT 31714-54-2P 94396-97-1P  
 RL: PREP (Preparation)  
 (isolation of, from pyrolysis of tetramethylsilane)

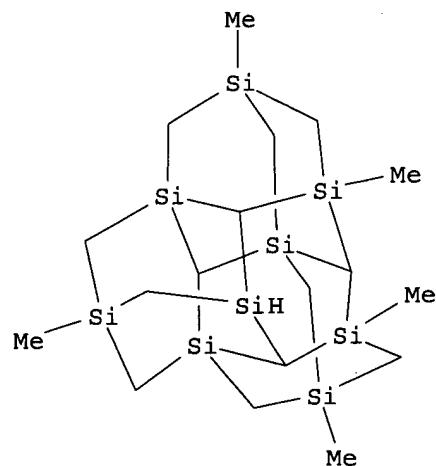
RN 31714-54-2 HCPLUS

CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-  
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-  
 2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)

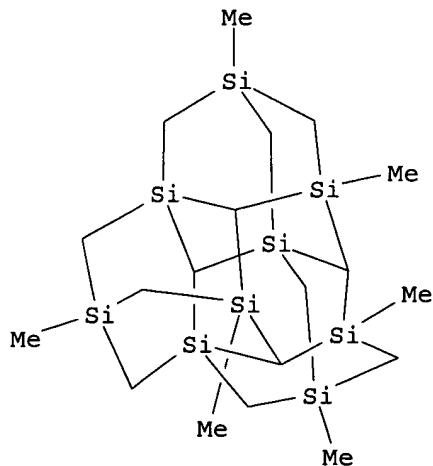


RN 94396-97-1 HCPLUS

CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-  
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9-  
 pentamethyl- (9CI) (CA INDEX NAME)



DN 73:56178  
 ED Entered STN: 12 May 1984  
 TI Silicon-carbon compounds with a carborundum structure ("carborundanes")  
 AU Fritz, Gerhard; Diem, Fritz; Koehler, Helmut; Kummer, Dieter; Scheer,  
 Heinz  
 CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.  
 SO Angewandte Chemie, International Edition in English (1970), 9(6), 464-5  
 CODEN: ACIEAY; ISSN: 0570-0833  
 DT Journal  
 LA English  
 CC 29 (Organometallic and Organometalloidal Compounds)  
 GI For diagram(s), see printed CA Issue.  
 AB 1,3,5,7-Tetramethyl-1,3,5,7-tetrasilatricyclo [3.3.1.13,7]decane (I) and  
 small amts. 1,3,7,9,11,13-hexamethyl-1,3,5,7,9,11,13-heptasilahexacyclo  
 [7.5.1.13,13.17,11.05,12.05,15]heptadecane (II), 3,7,11,13,15,17-  
 hexamethyl-1,3,5,7,9,11,13,15,17enneasilaenneacyclo  
 [9.1.7.11,5.13,17.17,15.05,16.09,14.09,20.013,18] docosane (III), and  
 3,7,11,17-tetramethyl-1,3,5,7,9,11,13,15,17,19-decasilaundecacyclo  
 [9.9.1.11,5.13.19.15,19.17,15.113,17.09,14.09,22.013,20.015,24]hexacosane  
 (IV) are obtained when SiMe<sub>4</sub> is pyrolyzed (700°). NMR data for  
 II-IV are given.  
 ST carborundanes silicon carbon compds; silicon carbon compds carborundanes;  
 carbon silicon compds carborundanes; silaadamantanes; adamantanes sila;  
 methyl silanes pyrolysis; silanes methyl pyrolysis; pyrolysis methyl  
 silanes  
 IT 26393-20-4P 31714-54-2P 32069-85-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 31714-54-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 31714-54-2 HCAPLUS  
 CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-  
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-  
 2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)



=&gt;